



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 20, 2025 – 08:15 PM JST

PDB ID : 9KAH / pdb_00009kah
Title : Crystal Structure of Chalcone Syntase and Chalcone Isomerase-like Protein Complex from *Physcomitrella patens*
Authors : Imaizumi, R.; Waki, T.; Yasuda, A.; Yanai, T.; Takeshita, K.; Sakai, N.; Yamamoto, M.; Nakayama, T.; Yamashita, S.
Deposited on : 2024-10-28
Resolution : 1.92 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

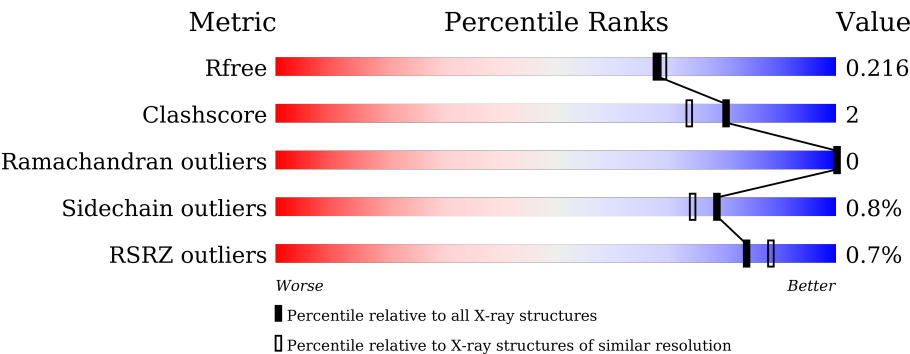
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.46

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.92 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1028 (1.92-1.92)
Clashscore	180529	1100 (1.92-1.92)
Ramachandran outliers	177936	1087 (1.92-1.92)
Sidechain outliers	177891	1087 (1.92-1.92)
RSRZ outliers	164620	1028 (1.92-1.92)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	413	<div><div></div><div></div><div></div><div></div><div></div><div></div></div> <div>90%6%</div>
1	B	413	<div><div></div><div></div><div></div><div></div><div></div><div></div></div> <div>88%6%6%</div>
1	E	413	<div><div></div><div></div><div></div><div></div><div></div><div></div></div> <div>%89%5%6%</div>
1	F	413	<div><div></div><div></div><div></div><div></div><div></div><div></div></div> <div>91%6%</div>
2	C	228	<div><div></div><div></div><div></div><div></div><div></div><div></div></div> <div>%78%13%9%</div>
2	D	228	<div><div></div><div></div><div></div><div></div><div></div><div></div></div> <div>%82%8%9%</div>

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Mol	Chain	Length	Quality of chain
2	G	228	<div><div></div><div>2%</div><div>84%</div><div>6%</div><div>10%</div></div>
2	H	228	<div><div></div><div>%</div><div>82%</div><div>8%</div><div>10%</div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 20998 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Chalcone synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	389	Total	C	N	O	S	0	4	0
			2974	1892	516	550	16			
1	B	387	Total	C	N	O	S	0	4	0
			2959	1884	511	548	16			
1	E	388	Total	C	N	O	S	0	4	0
			2962	1885	513	548	16			
1	F	388	Total	C	N	O	S	0	6	0
			2986	1900	517	553	16			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	MET	-	initiating methionine	UNP Q2VAZ3
A	-14	ASN	-	expression tag	UNP Q2VAZ3
A	-13	HIS	-	expression tag	UNP Q2VAZ3
A	-12	LYS	-	expression tag	UNP Q2VAZ3
A	-11	VAL	-	expression tag	UNP Q2VAZ3
A	-10	HIS	-	expression tag	UNP Q2VAZ3
A	-9	HIS	-	expression tag	UNP Q2VAZ3
A	-8	HIS	-	expression tag	UNP Q2VAZ3
A	-7	HIS	-	expression tag	UNP Q2VAZ3
A	-6	HIS	-	expression tag	UNP Q2VAZ3
A	-5	HIS	-	expression tag	UNP Q2VAZ3
A	-4	ILE	-	expression tag	UNP Q2VAZ3
A	-3	GLU	-	expression tag	UNP Q2VAZ3
A	-2	GLY	-	expression tag	UNP Q2VAZ3
A	-1	ARG	-	expression tag	UNP Q2VAZ3
A	0	HIS	-	expression tag	UNP Q2VAZ3
B	-15	MET	-	initiating methionine	UNP Q2VAZ3
B	-14	ASN	-	expression tag	UNP Q2VAZ3
B	-13	HIS	-	expression tag	UNP Q2VAZ3
B	-12	LYS	-	expression tag	UNP Q2VAZ3
B	-11	VAL	-	expression tag	UNP Q2VAZ3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-10	HIS	-	expression tag	UNP Q2VAZ3
B	-9	HIS	-	expression tag	UNP Q2VAZ3
B	-8	HIS	-	expression tag	UNP Q2VAZ3
B	-7	HIS	-	expression tag	UNP Q2VAZ3
B	-6	HIS	-	expression tag	UNP Q2VAZ3
B	-5	HIS	-	expression tag	UNP Q2VAZ3
B	-4	ILE	-	expression tag	UNP Q2VAZ3
B	-3	GLU	-	expression tag	UNP Q2VAZ3
B	-2	GLY	-	expression tag	UNP Q2VAZ3
B	-1	ARG	-	expression tag	UNP Q2VAZ3
B	0	HIS	-	expression tag	UNP Q2VAZ3
E	-15	MET	-	initiating methionine	UNP Q2VAZ3
E	-14	ASN	-	expression tag	UNP Q2VAZ3
E	-13	HIS	-	expression tag	UNP Q2VAZ3
E	-12	LYS	-	expression tag	UNP Q2VAZ3
E	-11	VAL	-	expression tag	UNP Q2VAZ3
E	-10	HIS	-	expression tag	UNP Q2VAZ3
E	-9	HIS	-	expression tag	UNP Q2VAZ3
E	-8	HIS	-	expression tag	UNP Q2VAZ3
E	-7	HIS	-	expression tag	UNP Q2VAZ3
E	-6	HIS	-	expression tag	UNP Q2VAZ3
E	-5	HIS	-	expression tag	UNP Q2VAZ3
E	-4	ILE	-	expression tag	UNP Q2VAZ3
E	-3	GLU	-	expression tag	UNP Q2VAZ3
E	-2	GLY	-	expression tag	UNP Q2VAZ3
E	-1	ARG	-	expression tag	UNP Q2VAZ3
E	0	HIS	-	expression tag	UNP Q2VAZ3
F	-15	MET	-	initiating methionine	UNP Q2VAZ3
F	-14	ASN	-	expression tag	UNP Q2VAZ3
F	-13	HIS	-	expression tag	UNP Q2VAZ3
F	-12	LYS	-	expression tag	UNP Q2VAZ3
F	-11	VAL	-	expression tag	UNP Q2VAZ3
F	-10	HIS	-	expression tag	UNP Q2VAZ3
F	-9	HIS	-	expression tag	UNP Q2VAZ3
F	-8	HIS	-	expression tag	UNP Q2VAZ3
F	-7	HIS	-	expression tag	UNP Q2VAZ3
F	-6	HIS	-	expression tag	UNP Q2VAZ3
F	-5	HIS	-	expression tag	UNP Q2VAZ3
F	-4	ILE	-	expression tag	UNP Q2VAZ3
F	-3	GLU	-	expression tag	UNP Q2VAZ3
F	-2	GLY	-	expression tag	UNP Q2VAZ3
F	-1	ARG	-	expression tag	UNP Q2VAZ3

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Chain	Residue	Modelled	Actual	Comment	Reference
F	0	HIS	-	expression tag	UNP Q2VAZ3

- Molecule 2 is a protein called Chalcone-flavonone isomerase family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	207	Total	C	N	O	S	0	1	0
			1615	1027	257	329	2			
2	D	208	Total	C	N	O	S	0	1	0
			1625	1032	262	329	2			
2	G	206	Total	C	N	O	S	0	2	0
			1609	1023	257	327	2			
2	H	206	Total	C	N	O	S	0	0	0
			1598	1016	255	325	2			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-15	MET	-	initiating methionine	UNP A9SRW1
C	-14	ASN	-	expression tag	UNP A9SRW1
C	-13	HIS	-	expression tag	UNP A9SRW1
C	-12	LYS	-	expression tag	UNP A9SRW1
C	-11	VAL	-	expression tag	UNP A9SRW1
C	-10	HIS	-	expression tag	UNP A9SRW1
C	-9	HIS	-	expression tag	UNP A9SRW1
C	-8	HIS	-	expression tag	UNP A9SRW1
C	-7	HIS	-	expression tag	UNP A9SRW1
C	-6	HIS	-	expression tag	UNP A9SRW1
C	-5	HIS	-	expression tag	UNP A9SRW1
C	-4	ILE	-	expression tag	UNP A9SRW1
C	-3	GLU	-	expression tag	UNP A9SRW1
C	-2	GLY	-	expression tag	UNP A9SRW1
C	-1	ARG	-	expression tag	UNP A9SRW1
C	0	HIS	-	expression tag	UNP A9SRW1
D	-15	MET	-	initiating methionine	UNP A9SRW1
D	-14	ASN	-	expression tag	UNP A9SRW1
D	-13	HIS	-	expression tag	UNP A9SRW1
D	-12	LYS	-	expression tag	UNP A9SRW1
D	-11	VAL	-	expression tag	UNP A9SRW1
D	-10	HIS	-	expression tag	UNP A9SRW1
D	-9	HIS	-	expression tag	UNP A9SRW1
D	-8	HIS	-	expression tag	UNP A9SRW1
D	-7	HIS	-	expression tag	UNP A9SRW1

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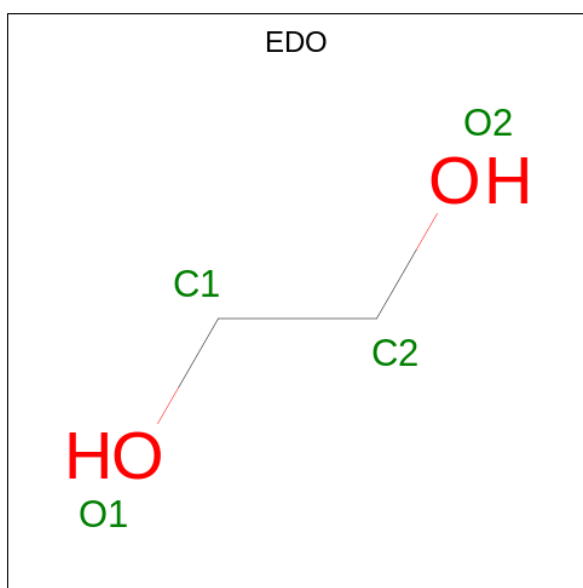
Chain	Residue	Modelled	Actual	Comment	Reference
D	-6	HIS	-	expression tag	UNP A9SRW1
D	-5	HIS	-	expression tag	UNP A9SRW1
D	-4	ILE	-	expression tag	UNP A9SRW1
D	-3	GLU	-	expression tag	UNP A9SRW1
D	-2	GLY	-	expression tag	UNP A9SRW1
D	-1	ARG	-	expression tag	UNP A9SRW1
D	0	HIS	-	expression tag	UNP A9SRW1
G	-15	MET	-	initiating methionine	UNP A9SRW1
G	-14	ASN	-	expression tag	UNP A9SRW1
G	-13	HIS	-	expression tag	UNP A9SRW1
G	-12	LYS	-	expression tag	UNP A9SRW1
G	-11	VAL	-	expression tag	UNP A9SRW1
G	-10	HIS	-	expression tag	UNP A9SRW1
G	-9	HIS	-	expression tag	UNP A9SRW1
G	-8	HIS	-	expression tag	UNP A9SRW1
G	-7	HIS	-	expression tag	UNP A9SRW1
G	-6	HIS	-	expression tag	UNP A9SRW1
G	-5	HIS	-	expression tag	UNP A9SRW1
G	-4	ILE	-	expression tag	UNP A9SRW1
G	-3	GLU	-	expression tag	UNP A9SRW1
G	-2	GLY	-	expression tag	UNP A9SRW1
G	-1	ARG	-	expression tag	UNP A9SRW1
G	0	HIS	-	expression tag	UNP A9SRW1
H	-15	MET	-	initiating methionine	UNP A9SRW1
H	-14	ASN	-	expression tag	UNP A9SRW1
H	-13	HIS	-	expression tag	UNP A9SRW1
H	-12	LYS	-	expression tag	UNP A9SRW1
H	-11	VAL	-	expression tag	UNP A9SRW1
H	-10	HIS	-	expression tag	UNP A9SRW1
H	-9	HIS	-	expression tag	UNP A9SRW1
H	-8	HIS	-	expression tag	UNP A9SRW1
H	-7	HIS	-	expression tag	UNP A9SRW1
H	-6	HIS	-	expression tag	UNP A9SRW1
H	-5	HIS	-	expression tag	UNP A9SRW1
H	-4	ILE	-	expression tag	UNP A9SRW1
H	-3	GLU	-	expression tag	UNP A9SRW1
H	-2	GLY	-	expression tag	UNP A9SRW1
H	-1	ARG	-	expression tag	UNP A9SRW1
H	0	HIS	-	expression tag	UNP A9SRW1

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			7	4	3		
3	H	1	Total	C	O	0	0
			7	4	3		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	G	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is water.

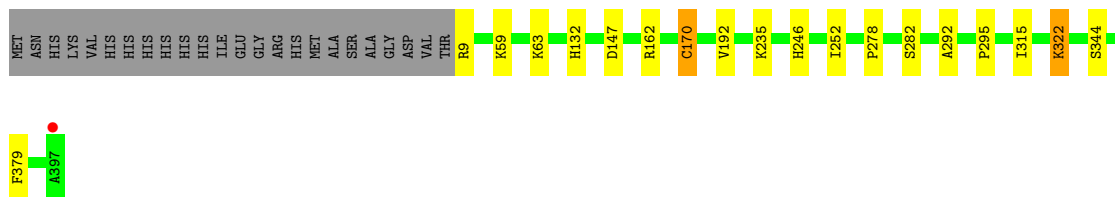
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	473	Total	O	0	0
			473	473		
5	B	479	Total	O	0	0
			479	479		
5	C	203	Total	O	0	0
			203	203		
5	D	190	Total	O	0	0
			190	190		
5	E	459	Total	O	0	0
			459	459		
5	F	426	Total	O	0	0
			426	426		
5	G	210	Total	O	0	0
			210	210		
5	H	204	Total	O	0	0
			204	204		

3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

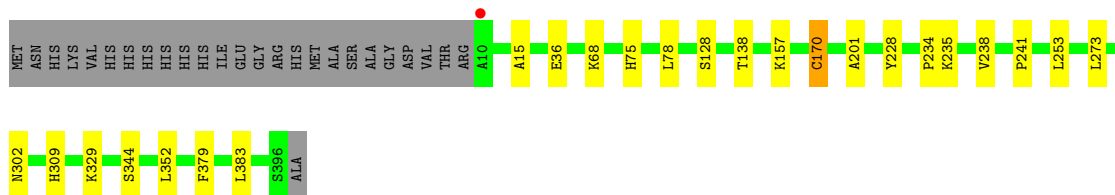
- Molecule 1: Chalcone synthase

Chain A: 




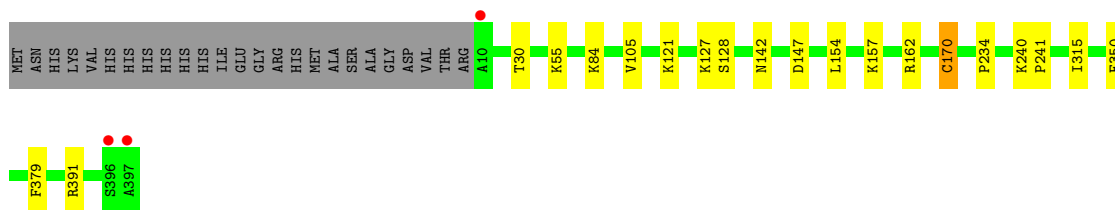
- Molecule 1: Chalcone synthase

Chain B: 




- Molecule 1: Chalcone synthase

Chain E: 




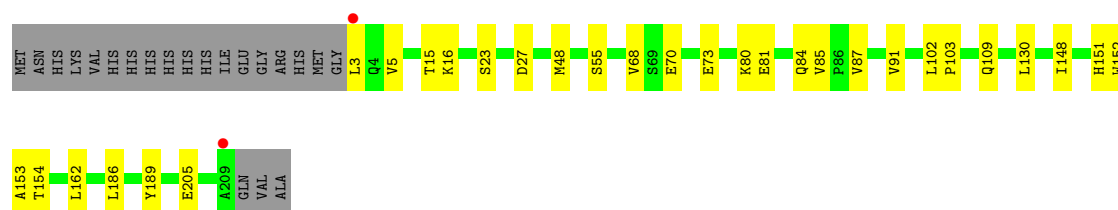
- Molecule 1: Chalcone synthase

Chain F: 




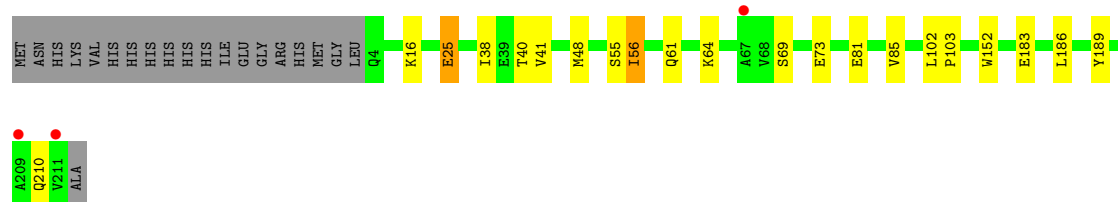
- Molecule 2: Chalcone-flavonone isomerase family protein

Chain C: 




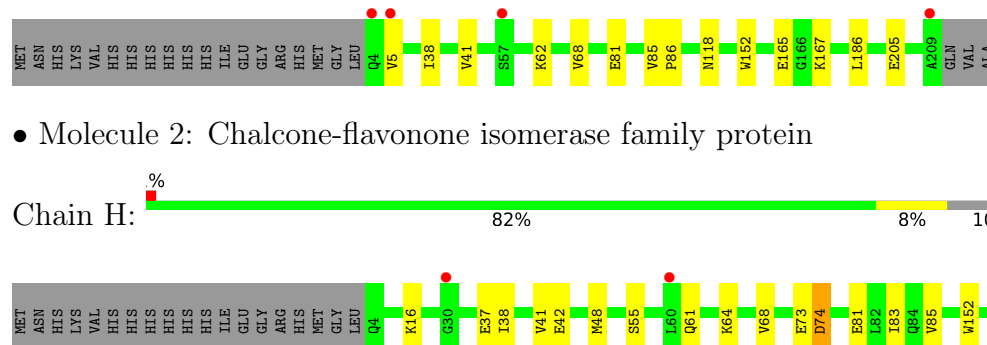
- Molecule 2: Chalcone-flavonone isomerase family protein

Chain D: 




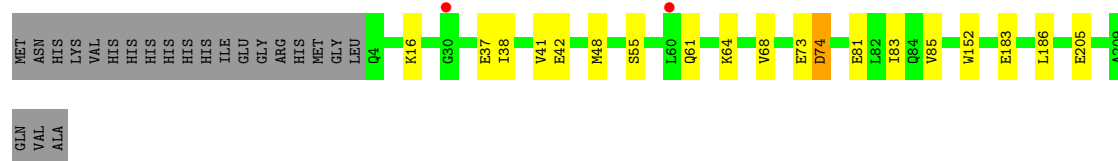
- Molecule 2: Chalcone-flavonone isomerase family protein

Chain G: 



- Molecule 2: Chalcone-flavonone isomerase family protein

Chain H: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	79.90Å 88.87Å 117.97Å 74.44° 74.32° 68.80°	Depositor
Resolution (Å)	49.19 – 1.92 49.19 – 1.92	Depositor EDS
% Data completeness (in resolution range)	99.0 (49.19-1.92) 99.0 (49.19-1.92)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 1.92Å)	Xtriage
Refinement program	PHENIX 1.21.2-5419, REFMAC 5.8.0430	Depositor
R, R_{free}	0.177 , 0.213 0.177 , 0.216	Depositor DCC
R_{free} test set	10913 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	28.9	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 41.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	20998	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.44% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, CSD, EDO

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.33	0/3023	0.48	0/4092
1	B	0.33	0/3008	0.50	0/4072
1	E	0.31	0/3011	0.48	0/4077
1	F	0.31	0/3035	0.47	0/4108
2	C	0.25	0/1646	0.44	0/2235
2	D	0.25	0/1656	0.45	0/2248
2	G	0.25	0/1640	0.44	0/2226
2	H	0.24	0/1629	0.46	0/2212
All	All	0.30	0/18648	0.47	0/25270

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2974	0	2999	11	0
1	B	2959	0	2983	15	0
1	E	2962	0	2986	14	0
1	F	2986	0	3009	11	0
2	C	1615	0	1586	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1625	0	1599	13	0
2	G	1609	0	1580	7	0
2	H	1598	0	1570	10	0
3	B	7	0	10	2	0
3	H	7	0	10	0	0
4	C	4	0	6	0	0
4	D	4	0	6	0	0
4	G	4	0	6	0	0
5	A	473	0	0	1	0
5	B	479	0	0	2	0
5	C	203	0	0	1	0
5	D	190	0	0	0	0
5	E	459	0	0	2	0
5	F	426	0	0	2	0
5	G	210	0	0	1	0
5	H	204	0	0	0	0
All	All	20998	0	18350	92	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (92) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:68:VAL:HG21	2:G:205:GLU:HG3	1.63	0.79
2:D:16:LYS:HG3	2:D:25:GLU:HG2	1.69	0.73
1:F:202:VAL:HG12	5:F:427:HOH:O	1.91	0.70
2:D:56:ILE:HD12	2:D:85:VAL:HG11	1.73	0.70
1:E:234:PRO:HG3	1:E:241:PRO:HG3	1.74	0.69
2:H:68:VAL:HG21	2:H:205:GLU:HG2	1.76	0.68
1:F:132:HIS:HB2	1:F:192:VAL:HG22	1.79	0.65
2:C:16:LYS:HE2	2:C:27:ASP:OD1	1.98	0.64
1:B:234:PRO:HG3	1:B:241:PRO:HG3	1.79	0.63
2:C:3:LEU:HD11	1:E:84:LYS:HE2	1.82	0.61
2:C:15:THR:C	2:C:16:LYS:HD2	2.29	0.58
2:C:152:TRP:CE2	2:C:186:LEU:HG	2.40	0.56
1:B:170[A]:CSD:HB3	1:B:379:PHE:O	2.05	0.56
2:H:61:GLN:HA	2:H:64:LYS:HD2	1.89	0.55
1:B:238:VAL:O	3:B:401:PEG:H11	2.07	0.54
2:C:70:GLU:O	2:C:73:GLU:HG2	2.07	0.54
2:H:81:GLU:O	2:H:85:VAL:HG23	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:81:GLU:O	2:D:85:VAL:HG23	2.08	0.52
1:B:170[B]:CSD:OD1	1:B:344[B]:SER:HA	2.11	0.51
2:G:118:ASN:HB2	5:G:538:HOH:O	2.09	0.51
1:A:282:SER:HB2	1:A:322:LYS:HG3	1.92	0.51
2:D:69:SER:O	2:D:73:GLU:HB2	2.11	0.51
2:C:80:LYS:O	2:C:84:GLN:HG2	2.12	0.50
2:D:61:GLN:HA	2:D:64:LYS:HD2	1.93	0.50
1:A:235:LYS:HB3	5:A:834:HOH:O	2.12	0.49
2:G:165:GLU:HG3	2:G:167:LYS:HD2	1.94	0.49
2:C:85:VAL:HG12	2:C:87:VAL:HG22	1.95	0.49
1:E:127:LYS:HD2	1:E:154:LEU:O	2.13	0.48
1:B:253:LEU:HD12	1:B:383[B]:LEU:HG	1.96	0.48
1:F:170[B]:CSD:HB3	1:F:379:PHE:O	2.14	0.48
2:D:64:LYS:HG2	2:D:210:GLN:HB2	1.94	0.48
1:A:278:PRO:HG3	1:A:315:ILE:HG13	1.96	0.47
1:E:147:ASP:OD2	1:E:162:ARG:HD2	2.14	0.47
1:E:128:SER:HB2	1:E:157:LYS:HE2	1.96	0.47
1:B:128:SER:HB2	1:B:157:LYS:HE3	1.96	0.47
1:E:391:ARG:CZ	1:F:9:ARG:HD2	2.45	0.47
1:F:68:LYS:HG2	5:F:479:HOH:O	2.14	0.46
2:H:73:GLU:HG3	2:H:74:ASP:N	2.30	0.46
2:H:38:ILE:O	2:H:41:VAL:HG12	2.16	0.46
2:H:73:GLU:HG3	2:H:74:ASP:H	1.81	0.46
1:F:127:LYS:HE2	1:F:127:LYS:HB2	1.77	0.45
2:G:38:ILE:O	2:G:41:VAL:HG12	2.16	0.45
1:B:273:LEU:HD13	2:D:38:ILE:CD1	2.47	0.45
2:G:81:GLU:O	2:G:85:VAL:HG23	2.16	0.45
1:E:55:LYS:NZ	5:E:401:HOH:O	2.34	0.45
2:G:152:TRP:CZ2	2:G:186:LEU:HD13	2.52	0.45
1:E:240:LYS:HB3	1:E:240:LYS:HE2	1.87	0.45
2:D:48:MET:HE1	2:D:189:TYR:CD1	2.52	0.44
1:A:132:HIS:HB2	1:A:192:VAL:HG22	1.99	0.44
2:H:37:GLU:HB2	2:H:42:GLU:OE2	2.18	0.44
2:D:102:LEU:HB3	2:D:103:PRO:HD3	2.00	0.44
1:E:170[A]:CSD:HB3	1:E:379:PHE:O	2.17	0.44
1:E:127:LYS:HB2	1:E:127:LYS:HE3	1.44	0.44
2:H:83:ILE:HG21	2:H:183:GLU:OE2	2.18	0.44
1:E:315:ILE:HG21	1:E:379:PHE:CZ	2.52	0.44
1:F:9:ARG:HA	1:F:9:ARG:HD3	1.85	0.43
2:C:102:LEU:HB3	2:C:103:PRO:HD3	2.01	0.43
2:D:152:TRP:CZ2	2:D:186:LEU:HD13	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:401:PEG:HG2	5:B:874:HOH:O	2.19	0.43
2:D:38:ILE:O	2:D:41:VAL:HG12	2.19	0.43
1:B:68:LYS:HG3	2:D:40:THR:HG21	2.00	0.43
1:A:170[A]:CSD:OD1	1:A:344[A]:SER:HA	2.20	0.42
1:B:228:TYR:HH	1:B:352:LEU:HB3	1.83	0.42
1:B:235:LYS:HB2	1:B:238:VAL:HB	2.00	0.42
2:G:85:VAL:HA	2:G:86:PRO:HD3	1.93	0.42
2:C:81:GLU:O	2:C:85:VAL:HG23	2.19	0.42
1:A:252:ILE:HD11	5:B:818:HOH:O	2.18	0.42
2:H:48:MET:HE2	2:H:48:MET:HB3	1.90	0.42
1:A:246:HIS:O	1:B:15:ALA:HB3	2.20	0.42
1:B:170[B]:CSD:HB2	1:B:309:HIS:NE2	2.35	0.42
1:B:302:ASN:HA	1:B:329:LYS:HE3	2.02	0.42
1:F:36:GLU:HG2	1:F:75:HIS:CE1	2.55	0.41
1:A:292:ALA:O	1:A:295:PRO:HD2	2.20	0.41
1:B:36:GLU:HG2	1:B:75:HIS:CE1	2.55	0.41
2:C:148:ILE:HG12	2:C:162:LEU:HD13	2.02	0.41
1:E:121:LYS:HD3	5:E:737:HOH:O	2.19	0.41
2:C:48:MET:HE1	2:C:189:TYR:CD1	2.55	0.41
2:C:151:HIS:CE1	2:C:153:ALA:HB2	2.56	0.41
2:C:68:VAL:HG21	2:C:205:GLU:HG3	2.02	0.41
1:F:315:ILE:HG21	1:F:379:PHE:CZ	2.56	0.41
1:F:30:THR:HB	1:F:350:PHE:CZ	2.56	0.41
1:A:147:ASP:OD2	1:A:162:ARG:HD2	2.21	0.40
1:A:315:ILE:HG21	1:A:379:PHE:CZ	2.55	0.40
2:C:23:SER:HA	5:C:541:HOH:O	2.21	0.40
1:E:105[A]:VAL:HG22	1:E:142:ASN:HB2	2.03	0.40
1:A:59:LYS:HG2	1:A:63:LYS:HE3	2.02	0.40
2:D:186:LEU:HD12	2:D:186:LEU:HA	1.97	0.40
1:F:170[A]:CSD:HB3	1:F:379:PHE:O	2.20	0.40
2:H:152:TRP:CE2	2:H:186:LEU:HD13	2.57	0.40
1:B:78:LEU:HD11	1:B:201:ALA:HA	2.02	0.40
2:C:109:GLN:HG3	2:C:130:LEU:HB3	2.02	0.40
1:E:30:THR:HB	1:E:350:PHE:CZ	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	389/413 (94%)	380 (98%)	9 (2%)	0	100	100
1	B	387/413 (94%)	374 (97%)	13 (3%)	0	100	100
1	E	388/413 (94%)	375 (97%)	13 (3%)	0	100	100
1	F	390/413 (94%)	379 (97%)	11 (3%)	0	100	100
2	C	206/228 (90%)	204 (99%)	2 (1%)	0	100	100
2	D	207/228 (91%)	204 (99%)	3 (1%)	0	100	100
2	G	206/228 (90%)	204 (99%)	2 (1%)	0	100	100
2	H	204/228 (90%)	198 (97%)	6 (3%)	0	100	100
All	All	2377/2564 (93%)	2318 (98%)	59 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	311/328 (95%)	309 (99%)	2 (1%)	84	80
1	B	310/328 (94%)	309 (100%)	1 (0%)	91	90
1	E	310/328 (94%)	310 (100%)	0	100	100
1	F	313/328 (95%)	313 (100%)	0	100	100
2	C	178/195 (91%)	174 (98%)	4 (2%)	47	32
2	D	179/195 (92%)	175 (98%)	4 (2%)	47	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	G	177/195 (91%)	175 (99%)	2 (1%)	70	63
2	H	176/195 (90%)	173 (98%)	3 (2%)	56	45
All	All	1954/2092 (93%)	1938 (99%)	16 (1%)	79	74

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ARG
1	A	322	LYS
1	B	138	THR
2	C	5	VAL
2	C	55	SER
2	C	91	VAL
2	C	154	THR
2	D	25	GLU
2	D	55	SER
2	D	56	ILE
2	D	183	GLU
2	G	5	VAL
2	G	62	LYS
2	H	16	LYS
2	H	55	SER
2	H	74	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	357	HIS
1	B	107	GLN
2	C	4	GLN
2	D	4	GLN
1	E	51	ASN
1	E	318	GLN
2	G	31	HIS
2	G	141	ASN
2	H	61	GLN
2	H	193	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

8 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	CSD	B	170[A]	1	3,7,8	0.42	0	1,8,10	7.08	1 (100%)
1	CSD	E	170[A]	1	3,7,8	0.51	0	1,8,10	7.78	1 (100%)
1	CSD	F	170[B]	1	3,7,8	0.47	0	1,8,10	8.59	1 (100%)
1	CSD	A	170[B]	1	3,7,8	0.54	0	1,8,10	7.66	1 (100%)
1	CSD	B	170[B]	1	3,7,8	0.60	0	1,8,10	8.83	1 (100%)
1	CSD	F	170[A]	1	3,7,8	0.33	0	1,8,10	8.39	1 (100%)
1	CSD	E	170[B]	1	3,7,8	0.53	0	1,8,10	7.72	1 (100%)
1	CSD	A	170[A]	1	3,7,8	0.63	0	1,8,10	7.58	1 (100%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSD	B	170[A]	1	-	1/2/6/8	-
1	CSD	E	170[A]	1	-	1/2/6/8	-
1	CSD	F	170[B]	1	-	1/2/6/8	-
1	CSD	A	170[B]	1	-	1/2/6/8	-
1	CSD	B	170[B]	1	-	0/2/6/8	-
1	CSD	F	170[A]	1	-	1/2/6/8	-
1	CSD	E	170[B]	1	-	0/2/6/8	-
1	CSD	A	170[A]	1	-	0/2/6/8	-

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	170[B]	CSD	OD1-SG-CB	8.83	122.34	105.54
1	F	170[B]	CSD	OD1-SG-CB	8.59	121.88	105.54
1	F	170[A]	CSD	OD1-SG-CB	8.39	121.50	105.54
1	E	170[A]	CSD	OD1-SG-CB	7.78	120.35	105.54
1	E	170[B]	CSD	OD1-SG-CB	7.72	120.22	105.54
1	A	170[B]	CSD	OD1-SG-CB	7.66	120.12	105.54
1	A	170[A]	CSD	OD1-SG-CB	7.58	119.97	105.54
1	B	170[A]	CSD	OD1-SG-CB	7.08	119.02	105.54

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	170[B]	CSD	CA-CB-SG-OD1
1	B	170[A]	CSD	CA-CB-SG-OD1
1	E	170[A]	CSD	CA-CB-SG-OD1
1	F	170[A]	CSD	CA-CB-SG-OD1
1	F	170[B]	CSD	CA-CB-SG-OD1

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	170[A]	CSD	1	0
1	E	170[A]	CSD	1	0
1	F	170[B]	CSD	1	0
1	B	170[B]	CSD	2	0
1	F	170[A]	CSD	1	0
1	A	170[A]	CSD	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	EDO	C	301	-	3,3,3	0.27	0	2,2,2	0.10	0
3	PEG	H	301	-	6,6,6	0.60	0	5,5,5	0.78	0
3	PEG	B	401	-	6,6,6	0.64	0	5,5,5	0.76	0
4	EDO	D	301	-	3,3,3	0.28	0	2,2,2	0.26	0
4	EDO	G	301	-	3,3,3	0.28	0	2,2,2	0.19	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	C	301	-	-	1/1/1/1	-
3	PEG	H	301	-	-	4/4/4/4	-
3	PEG	B	401	-	-	2/4/4/4	-
4	EDO	D	301	-	-	0/1/1/1	-
4	EDO	G	301	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	301	PEG	O2-C3-C4-O4
3	H	301	PEG	O1-C1-C2-O2
4	G	301	EDO	O1-C1-C2-O2
3	H	301	PEG	C4-C3-O2-C2
3	H	301	PEG	C1-C2-O2-C3
4	C	301	EDO	O1-C1-C2-O2
3	B	401	PEG	O2-C3-C4-O4
3	B	401	PEG	C4-C3-O2-C2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	401	PEG	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	388/413 (93%)	-0.64	1 (0%)	90	93	11, 25, 37, 86	3 (0%)
1	B	386/413 (93%)	-0.62	1 (0%)	90	93	11, 25, 43, 68	3 (0%)
1	E	387/413 (93%)	-0.56	3 (0%)	82	87	12, 27, 43, 67	3 (0%)
1	F	387/413 (93%)	-0.55	0	100	100	11, 27, 41, 66	5 (1%)
2	C	207/228 (90%)	-0.13	2 (0%)	79	84	17, 37, 60, 79	1 (0%)
2	D	208/228 (91%)	-0.01	3 (1%)	73	79	16, 39, 64, 75	1 (0%)
2	G	206/228 (90%)	-0.06	4 (1%)	66	72	12, 37, 60, 72	2 (0%)
2	H	206/228 (90%)	0.11	2 (0%)	79	84	25, 40, 65, 95	0
All	All	2375/2564 (92%)	-0.40	16 (0%)	84	88	11, 29, 56, 95	18 (0%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	3	LEU	4.0
1	A	397	ALA	3.5
2	G	4	GLN	3.1
2	D	211	VAL	2.9
1	B	10	ALA	2.8
2	G	209	ALA	2.6
1	E	10	ALA	2.5
2	H	60	LEU	2.2
2	D	67	ALA	2.1
2	G	5	VAL	2.1
1	E	396	SER	2.1
2	H	30	GLY	2.1
2	D	209	ALA	2.1
1	E	397	ALA	2.0
2	C	209	ALA	2.0
2	G	57	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	CSD	A	170[A]	8/9	0.94	0.08	22,23,27,28	8
1	CSD	A	170[B]	8/9	0.94	0.08	22,23,24,28	8
1	CSD	E	170[A]	8/9	0.95	0.09	25,27,35,36	8
1	CSD	E	170[B]	8/9	0.95	0.09	25,27,35,36	8
1	CSD	B	170[A]	8/9	0.97	0.07	22,22,27,31	8
1	CSD	B	170[B]	8/9	0.97	0.07	22,24,26,26	8
1	CSD	F	170[A]	8/9	0.97	0.06	23,24,30,31	8
1	CSD	F	170[B]	8/9	0.97	0.06	23,24,30,30	8

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	PEG	B	401	7/7	0.83	0.14	47,52,54,58	0
4	EDO	G	301	4/4	0.86	0.12	40,44,48,54	0
4	EDO	D	301	4/4	0.89	0.11	46,48,49,54	0
3	PEG	H	301	7/7	0.90	0.10	51,61,62,63	0
4	EDO	C	301	4/4	0.92	0.09	37,47,50,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.