



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 19, 2024 – 02:09 AM EDT

PDB ID : 3VYU
Title : Crystal structure of the HypC-HypD-HypE complex (form II)
Authors : Watanabe, S.; Miki, K.
Deposited on : 2012-10-02
Resolution : 2.75 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 : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.20.1
EDS : 2.37.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

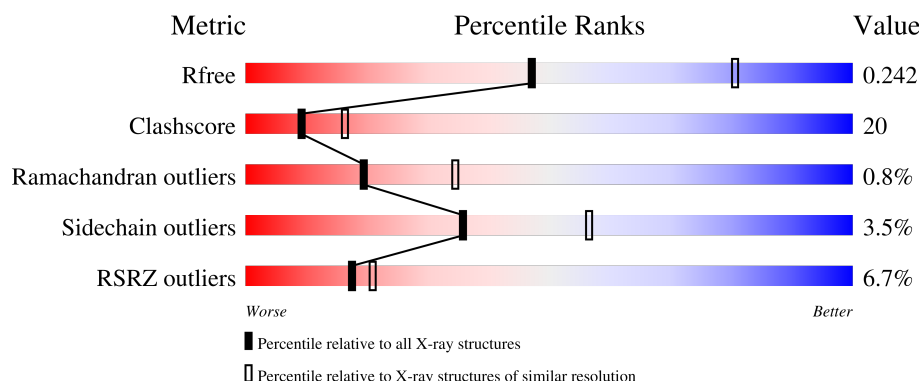
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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}	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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	74	<div> <div>15%</div> <div>30% 42% 27%</div> </div>
2	B	372	<div> <div>6%</div> <div>61% 36%</div> </div>
3	C	338	<div> <div>5%</div> <div>63% 25% 10%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SF4	B	501	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5489 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 Hydrogenase expression/formation protein HypC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	54	Total	C	N	O	S	0	0	0
			387	250	63	73	1			

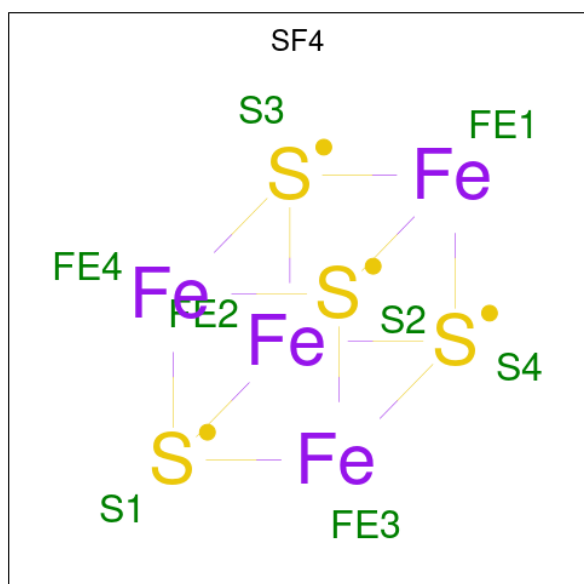
- Molecule 2 is a protein called Hydrogenase expression/formation protein HypD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	367	Total	C	N	O	S	0	0	0
			2835	1824	475	515	21			

- Molecule 3 is a protein called Hydrogenase expression/formation protein HypE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	305	Total	C	N	O	S	0	0	0
			2249	1417	385	436	11			

- Molecule 4 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



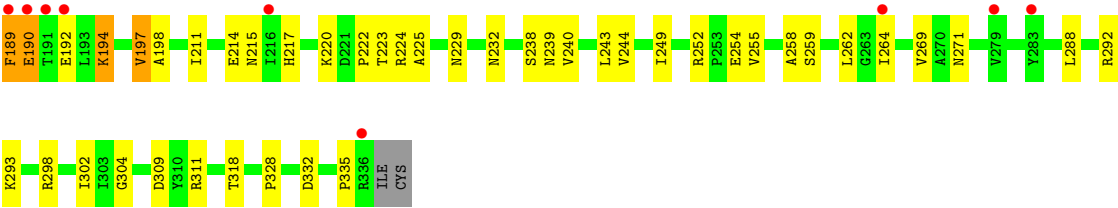
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total	O	0	0
			2	2		
5	C	8	Total	O	0	0
			8	8		

- Molecule 1: Hydrogenase expression/formation protein HypC





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	114.68Å 121.46Å 67.35Å 90.00° 97.20° 90.00°	Depositor
Resolution (Å)	36.81 – 2.75 49.88 – 2.75	Depositor EDS
% Data completeness (in resolution range)	88.6 (36.81-2.75) 88.6 (49.88-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 2.77Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.219 , 0.258 0.209 , 0.242	Depositor DCC
R_{free} test set	1069 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	80.6	Xtriage
Anisotropy	0.451	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 83.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5489	wwPDB-VP
Average B, all atoms (Å ²)	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.69% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4

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	0.30	0/395	0.62	0/542
2	B	0.32	0/2899	0.58	0/3934
3	C	0.34	0/2282	0.62	0/3095
All	All	0.33	0/5576	0.60	0/7571

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

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	387	0	369	31	0
2	B	2835	0	2817	114	0
3	C	2249	0	2260	80	0
4	B	8	0	0	2	0
5	B	2	0	0	0	0
5	C	8	0	0	0	0
All	All	5489	0	5446	217	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 20.

All (217) 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)
3:C:184:ARG:NH2	3:C:184:ARG:HB3	1.71	1.06
3:C:184:ARG:NH2	3:C:184:ARG:CB	2.21	1.02
3:C:184:ARG:HB2	3:C:184:ARG:CZ	1.90	1.01
2:B:134:ALA:HA	2:B:142:VAL:HG11	1.40	1.00
3:C:184:ARG:HB3	3:C:184:ARG:HH21	1.25	0.94
2:B:294:GLU:HG2	2:B:295:LEU:HD22	1.51	0.91
3:C:21:ARG:HG2	3:C:23:VAL:HG23	1.54	0.89
3:C:169:VAL:HG21	3:C:173:ILE:HD11	1.55	0.89
3:C:262:LEU:O	3:C:335:PRO:HA	1.72	0.88
2:B:295:LEU:HG	2:B:303:GLU:HB2	1.62	0.82
2:B:295:LEU:HD22	2:B:295:LEU:H	1.45	0.79
3:C:184:ARG:CB	3:C:184:ARG:CZ	2.55	0.77
2:B:154:ALA:HB3	2:B:155:PRO:HD3	1.67	0.76
2:B:180:THR:HB	2:B:181:PRO:HD3	1.68	0.75
2:B:295:LEU:HD22	2:B:295:LEU:N	2.01	0.75
2:B:264:ASN:O	2:B:268:GLN:HG3	1.87	0.74
3:C:184:ARG:CB	3:C:184:ARG:HH21	1.89	0.73
2:B:174:TYR:CZ	2:B:305:ARG:HD3	2.25	0.71
1:A:45:HIS:CD2	2:B:151:THR:HG22	2.25	0.70
3:C:107:MET:HE2	3:C:107:MET:HA	1.74	0.70
2:B:257:ARG:HG2	2:B:257:ARG:HH11	1.57	0.70
3:C:288:LEU:HD22	3:C:302:ILE:HG13	1.73	0.69
2:B:10:SER:HB3	2:B:13:VAL:HG23	1.76	0.68
2:B:86:ALA:HA	2:B:308:TYR:HE1	1.59	0.68
2:B:158:GLY:HA2	2:B:270:MET:SD	2.37	0.65
3:C:75:ARG:HG3	3:C:120:THR:OG1	1.97	0.65
3:C:223:THR:OG1	3:C:224:ARG:N	2.30	0.65
3:C:55:VAL:HG21	3:C:90:ALA:HB2	1.78	0.64
2:B:294:GLU:HG2	2:B:295:LEU:CD2	2.25	0.63
3:C:46:THR:HG23	3:C:53:HIS:HB3	1.80	0.63
3:C:254:GLU:OE2	3:C:254:GLU:N	2.32	0.62
2:B:295:LEU:CG	2:B:303:GLU:HB2	2.29	0.62
1:A:24:VAL:HG13	3:C:187:ILE:HG23	1.81	0.62
4:B:501:SF4:FE2	4:B:501:SF4:S4	1.91	0.62
4:B:501:SF4:FE2	4:B:501:SF4:S3	1.92	0.62
1:A:23:GLY:HA3	3:C:189:PHE:CE1	2.36	0.61
1:A:29:ARG:HD3	2:B:128:PHE:CE1	2.36	0.60
3:C:93:ILE:HG13	3:C:151:ILE:HG12	1.83	0.60
1:A:30:LEU:HD22	1:A:33:MET:O	2.00	0.60
2:B:174:TYR:CE1	2:B:305:ARG:HD3	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:38:CYS:HB2	2:B:200:PRO:HB3	1.83	0.60
3:C:145:ILE:N	3:C:145:ILE:HD12	2.17	0.60
3:C:181:MET:HG2	3:C:262:LEU:HD13	1.84	0.60
2:B:273:LYS:HE2	2:B:299:TRP:CZ2	2.36	0.59
3:C:124:VAL:HB	3:C:125:PRO:C	2.23	0.59
2:B:157:ALA:HB2	2:B:275:PHE:HE1	1.67	0.59
3:C:44:GLY:HA3	3:C:88:MET:SD	2.42	0.59
3:C:262:LEU:O	3:C:335:PRO:CA	2.48	0.58
2:B:143:VAL:HG22	2:B:172:LYS:HB2	1.84	0.58
3:C:222:PRO:O	3:C:271:ASN:HB2	2.03	0.58
3:C:225:ALA:HB1	3:C:229:ASN:HB2	1.84	0.58
1:A:21:PHE:HZ	1:A:44:VAL:HG21	1.69	0.58
2:B:205:THR:HG22	2:B:206:ILE:HD13	1.86	0.57
2:B:273:LYS:HD3	2:B:274:PHE:CE1	2.38	0.57
1:A:37:LYS:HG2	1:A:40:ASP:OD2	2.03	0.57
1:A:32:LEU:HB2	1:A:49:ALA:O	2.04	0.57
2:B:295:LEU:CD2	2:B:303:GLU:HB2	2.34	0.57
1:A:8:LYS:HB2	1:A:41:TRP:CZ2	2.40	0.57
2:B:237:ILE:O	2:B:241:ILE:HG13	2.05	0.56
1:A:4:ALA:HB3	2:B:202:HIS:CE1	2.40	0.56
2:B:257:ARG:HG2	2:B:257:ARG:NH1	2.20	0.56
2:B:142:VAL:HG13	2:B:170:ASN:O	2.05	0.56
1:A:54:ASP:OD2	1:A:55:GLU:N	2.38	0.56
1:A:43:ILE:HD11	2:B:258:ALA:HB1	1.87	0.56
2:B:213:GLU:HA	2:B:251:ILE:HD11	1.88	0.56
3:C:244:VAL:HG11	3:C:249:ILE:HD11	1.88	0.56
3:C:174:GLY:HA2	3:C:269:VAL:HG23	1.86	0.55
2:B:135:LYS:O	2:B:138:PRO:HD3	2.06	0.55
2:B:200:PRO:HG2	2:B:203:VAL:HB	1.87	0.55
1:A:16:VAL:HG12	1:A:16:VAL:O	2.05	0.55
2:B:134:ALA:CA	2:B:142:VAL:HG11	2.26	0.55
2:B:8:TYR:HB3	2:B:229:GLU:HG3	1.88	0.55
2:B:168:LEU:HD23	2:B:169:GLU:H	1.71	0.54
2:B:153:THR:HG21	2:B:293:LEU:HD23	1.89	0.54
2:B:295:LEU:HD21	2:B:303:GLU:CG	2.37	0.54
2:B:280:ALA:HB2	2:B:292:GLY:HA3	1.89	0.53
2:B:265:VAL:HA	2:B:268:GLN:OE1	2.08	0.53
3:C:224:ARG:O	3:C:225:ALA:HB3	2.09	0.53
2:B:209:VAL:CG2	2:B:253:ASN:HD22	2.21	0.53
2:B:180:THR:HG22	2:B:212:TRP:HH2	1.74	0.53
3:C:160:GLY:O	3:C:217:HIS:HB3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:189:PHE:CZ	3:C:254:GLU:HA	2.43	0.53
2:B:83:MET:HG3	2:B:114:LEU:HD21	1.92	0.52
3:C:65:PRO:HG2	3:C:67:PHE:O	2.09	0.52
1:A:44:VAL:HA	1:A:48:PHE:O	2.09	0.52
2:B:150:GLU:OE1	2:B:203:VAL:HG13	2.10	0.52
3:C:214:GLU:CD	3:C:214:GLU:H	2.13	0.52
2:B:73:VAL:HG23	2:B:74:GLU:N	2.24	0.51
2:B:181:PRO:HB2	2:B:182:PRO:HD3	1.92	0.51
3:C:61:HIS:NE2	3:C:77:ALA:HA	2.25	0.51
3:C:184:ARG:NH2	3:C:184:ARG:HB2	1.99	0.51
3:C:107:MET:HA	3:C:107:MET:CE	2.41	0.51
1:A:12:VAL:HG23	1:A:38:PRO:HG3	1.92	0.51
3:C:178:ILE:HG13	3:C:255:VAL:HG13	1.94	0.50
2:B:150:GLU:OE2	2:B:179:LEU:HA	2.10	0.50
2:B:137:ASN:N	2:B:138:PRO:HD3	2.27	0.50
2:B:354:CYS:HB3	2:B:362:CYS:SG	2.52	0.50
3:C:177:GLY:HA3	3:C:269:VAL:HB	1.93	0.50
1:A:20:ASP:HA	1:A:24:VAL:O	2.11	0.50
3:C:167:VAL:C	3:C:168:LEU:HD12	2.32	0.50
1:A:19:VAL:HG12	1:A:20:ASP:N	2.27	0.50
2:B:235:MET:O	2:B:239:MET:HG3	2.12	0.50
3:C:211:ILE:O	3:C:215:ASN:ND2	2.34	0.50
3:C:185:GLU:HA	3:C:185:GLU:OE1	2.12	0.49
2:B:150:GLU:HG2	2:B:207:ILE:CG2	2.42	0.49
2:B:276:GLU:HB3	2:B:296:ARG:HG2	1.94	0.49
3:C:101:ILE:HG23	3:C:105:LEU:HD22	1.94	0.49
2:B:292:GLY:O	2:B:293:LEU:HD12	2.12	0.49
2:B:28:LEU:HD23	2:B:29:ASP:N	2.28	0.49
2:B:146:SER:HG	2:B:177:HIS:CE1	2.31	0.49
2:B:295:LEU:HD21	2:B:303:GLU:OE2	2.13	0.49
2:B:168:LEU:HD23	2:B:169:GLU:N	2.28	0.48
2:B:157:ALA:HB2	2:B:275:PHE:CE1	2.47	0.48
2:B:335:PRO:HB3	2:B:362:CYS:SG	2.53	0.48
3:C:225:ALA:CB	3:C:229:ASN:HB2	2.43	0.48
3:C:259:SER:HB2	3:C:264:ILE:O	2.12	0.48
2:B:79:MET:O	2:B:83:MET:HG2	2.12	0.48
3:C:55:VAL:CG2	3:C:90:ALA:HB2	2.43	0.48
2:B:86:ALA:HA	2:B:308:TYR:CE1	2.46	0.48
2:B:100:ASP:OD1	2:B:101:MET:N	2.47	0.48
2:B:335:PRO:HG2	2:B:365:PHE:CG	2.48	0.48
3:C:105:LEU:HD13	3:C:141:GLU:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:313:PRO:HG2	2:B:316:LEU:HD11	1.95	0.47
2:B:145:PHE:O	2:B:147:PRO:HD3	2.14	0.47
3:C:258:ALA:O	3:C:262:LEU:HG	2.14	0.47
2:B:37:VAL:CG2	2:B:200:PRO:HD3	2.45	0.47
2:B:295:LEU:N	2:B:295:LEU:CD2	2.72	0.47
2:B:314:LYS:O	2:B:315:ASN:HB2	2.14	0.47
3:C:140:ILE:O	3:C:141:GLU:HB2	2.14	0.47
3:C:244:VAL:CG1	3:C:249:ILE:HD11	2.43	0.47
2:B:365:PHE:CD2	2:B:370:VAL:HG11	2.50	0.47
3:C:239:ASN:O	3:C:311:ARG:HD3	2.15	0.47
2:B:332:LEU:O	2:B:333:ALA:HB2	2.14	0.46
3:C:232:ASN:ND2	3:C:328:PRO:HD3	2.30	0.46
1:A:8:LYS:NZ	1:A:8:LYS:HB3	2.29	0.46
2:B:66:CYS:O	2:B:70:ILE:HG13	2.15	0.46
2:B:204:SER:HG	2:B:212:TRP:HE1	1.63	0.46
1:A:37:LYS:NZ	1:A:39:GLY:HA3	2.30	0.46
2:B:10:SER:HB3	2:B:13:VAL:CG2	2.43	0.46
3:C:99:MET:HE2	3:C:144:VAL:HG22	1.97	0.46
3:C:107:MET:CE	3:C:107:MET:CA	2.94	0.46
3:C:124:VAL:HB	3:C:125:PRO:CA	2.46	0.46
3:C:243:LEU:O	3:C:304:GLY:HA3	2.16	0.45
1:A:43:ILE:CD1	2:B:258:ALA:HB1	2.47	0.45
2:B:8:TYR:O	2:B:229:GLU:HB3	2.17	0.45
3:C:168:LEU:HG	3:C:302:ILE:HG12	1.99	0.45
3:C:68:PHE:CG	3:C:180:LEU:HD11	2.52	0.45
2:B:162:VAL:HG12	2:B:162:VAL:O	2.17	0.45
1:A:9:VAL:O	1:A:38:PRO:O	2.35	0.45
3:C:187:ILE:HD12	3:C:262:LEU:HD21	1.98	0.45
1:A:8:LYS:HB2	1:A:41:TRP:CE2	2.51	0.44
2:B:262:GLU:CD	2:B:262:GLU:H	2.20	0.44
2:B:308:TYR:N	2:B:308:TYR:CD2	2.86	0.44
2:B:132:ARG:O	2:B:136:GLU:HG3	2.17	0.44
2:B:152:THR:HG22	2:B:152:THR:O	2.16	0.44
2:B:186:VAL:O	2:B:190:GLN:HG3	2.18	0.44
2:B:122:ARG:HH11	2:B:133:ILE:HD13	1.83	0.44
2:B:343:LYS:HB2	2:B:344:THR:H	1.63	0.44
3:C:21:ARG:CG	3:C:23:VAL:HG23	2.37	0.44
2:B:96:THR:HA	2:B:122:ARG:O	2.18	0.43
3:C:172:THR:HG21	3:C:252:ARG:HG3	1.99	0.43
3:C:174:GLY:HA2	3:C:269:VAL:CG2	2.48	0.43
2:B:150:GLU:HG2	2:B:207:ILE:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:365:PHE:HD2	2:B:370:VAL:HG11	1.84	0.43
3:C:51:ASP:OD1	3:C:52:LYS:HG2	2.18	0.43
2:B:243:MET:CE	2:B:252:ILE:HD12	2.48	0.43
2:B:168:LEU:HD21	2:B:170:ASN:OD1	2.19	0.43
2:B:221:ILE:O	2:B:221:ILE:HG13	2.17	0.43
3:C:197:VAL:HG13	3:C:197:VAL:O	2.18	0.43
1:A:11:GLU:HB2	1:A:18:VAL:HB	2.00	0.43
2:B:21:ILE:HG23	2:B:241:ILE:CD1	2.49	0.43
1:A:24:VAL:HG22	3:C:189:PHE:CE2	2.54	0.43
1:A:37:LYS:HZ3	1:A:39:GLY:HA3	1.84	0.43
2:B:14:ALA:O	2:B:18:VAL:HG23	2.19	0.43
2:B:34:ILE:HG23	2:B:240:LEU:HD13	2.01	0.43
2:B:84:ARG:HH11	2:B:84:ARG:HG2	1.83	0.43
2:B:73:VAL:CG2	2:B:74:GLU:N	2.81	0.43
1:A:9:VAL:HG23	1:A:40:ASP:O	2.19	0.42
3:C:252:ARG:HH11	3:C:252:ARG:HG2	1.84	0.42
3:C:197:VAL:O	3:C:198:ALA:HB2	2.19	0.42
1:A:17:ALA:HB2	1:A:30:LEU:HD11	2.01	0.42
2:B:48:HIS:HA	3:C:318:THR:HG21	2.02	0.42
2:B:127:ILE:O	2:B:130:THR:HB	2.19	0.42
2:B:178:ARG:CZ	2:B:280:ALA:HB1	2.50	0.42
3:C:145:ILE:N	3:C:145:ILE:CD1	2.83	0.42
1:A:23:GLY:HA2	3:C:190:GLU:OE1	2.19	0.42
2:B:175:SER:OG	2:B:293:LEU:O	2.29	0.42
3:C:117:MET:HB3	3:C:117:MET:HE2	1.66	0.42
2:B:9:ARG:HG2	2:B:229:GLU:OE1	2.20	0.42
2:B:83:MET:HG3	2:B:114:LEU:CD2	2.50	0.42
3:C:238:SER:O	3:C:240:VAL:HG13	2.20	0.42
2:B:87:ARG:C	2:B:89:GLU:H	2.22	0.42
2:B:188:LEU:HD11	2:B:221:ILE:HD13	2.01	0.42
3:C:106:ASP:O	3:C:109:VAL:HB	2.20	0.42
1:A:28:VAL:HG21	1:A:44:VAL:HG21	2.02	0.41
2:B:93:ILE:HG23	2:B:141:THR:O	2.21	0.41
3:C:292:ARG:NH1	3:C:298:ARG:O	2.53	0.41
2:B:324:ARG:O	2:B:328:VAL:HG23	2.20	0.41
2:B:270:MET:O	2:B:273:LYS:HB3	2.20	0.41
3:C:107:MET:HE2	3:C:107:MET:CA	2.47	0.41
2:B:33:ARG:HH21	2:B:193:VAL:HG13	1.85	0.41
2:B:180:THR:HB	2:B:181:PRO:CD	2.46	0.41
1:A:21:PHE:HZ	1:A:44:VAL:CG2	2.32	0.41
2:B:153:THR:HG21	2:B:293:LEU:CD2	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:192:GLU:OE1	3:C:194:LYS:HD2	2.21	0.41
2:B:6:GLU:O	2:B:10:SER:N	2.52	0.41
2:B:299:TRP:C	2:B:301:ASP:H	2.23	0.41
3:C:169:VAL:CG2	3:C:173:ILE:HD11	2.37	0.41
2:B:338:CYS:HA	2:B:339:PRO:HD2	1.88	0.40
1:A:33:MET:CE	1:A:51:GLU:HA	2.50	0.40
3:C:97:ASN:OD1	3:C:117:MET:HE3	2.21	0.40
3:C:105:LEU:O	3:C:106:ASP:C	2.60	0.40
2:B:14:ALA:HB2	2:B:231:ASN:HD21	1.86	0.40
2:B:143:VAL:HG21	2:B:304:ILE:HD13	2.03	0.40
2:B:154:ALA:HB3	2:B:155:PRO:CD	2.44	0.40
3:C:68:PHE:CD1	3:C:180:LEU:HD11	2.55	0.40
3:C:90:ALA:HA	3:C:152:ALA:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	52/74 (70%)	45 (86%)	6 (12%)	1 (2%)	8	14
2	B	365/372 (98%)	334 (92%)	30 (8%)	1 (0%)	41	60
3	C	301/338 (89%)	278 (92%)	19 (6%)	4 (1%)	12	21
All	All	718/784 (92%)	657 (92%)	55 (8%)	6 (1%)	19	34

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	208	GLY
1	A	16	VAL
3	C	141	GLU
3	C	190	GLU

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Mol	Chain	Res	Type
3	C	197	VAL
3	C	187	ILE

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	39/60 (65%)	38 (97%)	1 (3%)	46	66
2	B	300/319 (94%)	289 (96%)	11 (4%)	34	54
3	C	233/265 (88%)	225 (97%)	8 (3%)	37	58
All	All	572/644 (89%)	552 (96%)	20 (4%)	36	56

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	VAL
2	B	19	GLU
2	B	61	VAL
2	B	139	ASP
2	B	142	VAL
2	B	168	LEU
2	B	176	VAL
2	B	214	TYR
2	B	265	VAL
2	B	295	LEU
2	B	308	TYR
2	B	344	THR
3	C	175	ASP
3	C	184	ARG
3	C	189	PHE
3	C	194	LYS
3	C	220	LYS
3	C	293	LYS
3	C	309	ASP
3	C	332	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	202	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	SF4	B	501	2	0,12,12	-	-	-		

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	SF4	B	501	2	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	501	SF4	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	54/74 (72%)	0.97	11 (20%) 1 1	120, 140, 149, 152	0
2	B	367/372 (98%)	0.49	22 (5%) 21 26	81, 109, 143, 172	0
3	C	305/338 (90%)	0.55	16 (5%) 27 33	73, 97, 154, 167	0
All	All	726/784 (92%)	0.55	49 (6%) 17 21	73, 106, 147, 172	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	24	ILE	9.3
1	A	53	LEU	5.7
3	C	25	LEU	5.0
3	C	336	ARG	4.4
1	A	8	LYS	4.2
3	C	43	ASP	4.2
2	B	371	LEU	4.1
3	C	41	LEU	3.9
1	A	50	ILE	3.8
2	B	114	LEU	3.7
2	B	83	MET	3.7
1	A	51	GLU	3.7
2	B	192	THR	3.6
3	C	44	GLY	3.5
2	B	194	PHE	3.3
2	B	108	MET	3.2
3	C	216	ILE	2.9
3	C	192	GLU	2.9
1	A	41	TRP	2.9
3	C	27	THR	2.9
2	B	202	HIS	2.7
2	B	308	TYR	2.7
1	A	21	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	119	PHE	2.6
2	B	140	LYS	2.5
2	B	90	GLY	2.5
2	B	252	ILE	2.5
2	B	313	PRO	2.5
1	A	39	GLY	2.5
3	C	40	ALA	2.5
2	B	82	ILE	2.4
3	C	279	VAL	2.4
1	A	42	VAL	2.4
2	B	316	LEU	2.4
2	B	8	TYR	2.4
2	B	85	LYS	2.3
2	B	28	LEU	2.3
2	B	241	ILE	2.3
3	C	189	PHE	2.3
1	A	7	GLY	2.2
3	C	283	TYR	2.2
2	B	159	MET	2.2
2	B	319	LEU	2.2
3	C	264	ILE	2.2
2	B	95	LEU	2.1
1	A	43	ILE	2.1
3	C	191	THR	2.1
1	A	40	ASP	2.1
3	C	190	GLU	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no monosaccharides 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(\AA^2)	Q<0.9
4	SF4	B	501	8/8	0.99	0.21	99,101,110,111	0

6.5 Other polymers [i](#)

There are no such residues in this entry.