



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 2, 2024 – 09:22 AM EST

PDB ID : 1D0G
Title : CRYSTAL STRUCTURE OF DEATH RECEPTOR 5 (DR5) BOUND TO APO2L/TRAIL
Authors : Hymowitz, S.G.; Christinger, H.W.; Fuh, G.; O'Connell, M.P.; Kelley, R.F.; Ashkenazi, A.; de Vos, A.M.
Deposited on : 1999-09-09
Resolution : 2.40 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
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

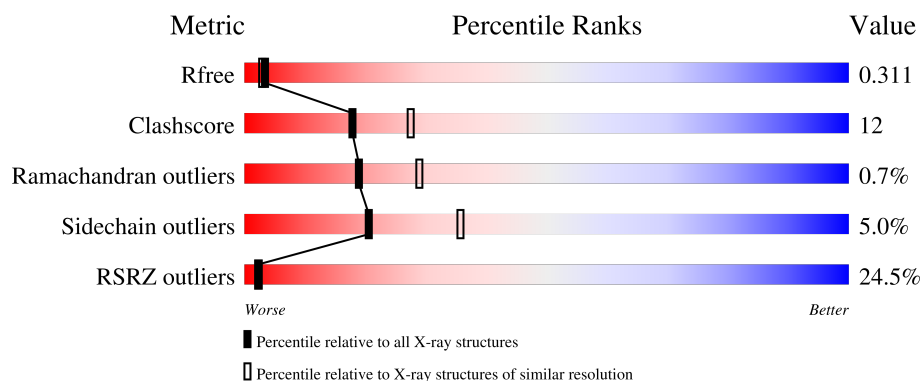
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4642 (2.40-2.40)
Clashscore	180529	5218 (2.40-2.40)
Ramachandran outliers	177936	5158 (2.40-2.40)
Sidechain outliers	177891	5159 (2.40-2.40)
RSRZ outliers	164620	4642 (2.40-2.40)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	R	130	<div> <div>11%</div> <div>58%</div> <div>24%</div> <div>•</div> <div>17%</div> </div>
1	S	130	<div> <div>42%</div> <div>65%</div> <div>17%</div> <div>•</div> <div>15%</div> </div>
1	T	130	<div> <div>25%</div> <div>55%</div> <div>26%</div> <div>•</div> <div>15%</div> </div>
2	A	168	<div> <div>16%</div> <div>67%</div> <div>20%</div> <div>•</div> <div>10%</div> </div>
2	B	168	<div> <div>24%</div> <div>67%</div> <div>22%</div> <div>•</div> <div>10%</div> </div>
2	D	168	<div> <div>14%</div> <div>69%</div> <div>19%</div> <div>••</div> <div>10%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6576 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 DEATH RECEPTOR-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	R	108	Total	C	N	O	S	0	0	0
			833	498	150	169	16			
1	S	110	Total	C	N	O	S	0	0	0
			849	506	152	175	16			
1	T	110	Total	C	N	O	S	0	0	0
			849	506	152	175	16			

- Molecule 2 is a protein called APOPTOSIS-2 LIGAND.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	151	Total	C	N	O	S	8	1	0
			1253	800	216	233	4			
2	B	151	Total	C	N	O	S	16	1	0
			1253	800	216	233	4			
2	D	151	Total	C	N	O	S	16	1	0
			1253	800	216	233	4			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Cl	0	0
			1	1		

- Molecule 5 is water.

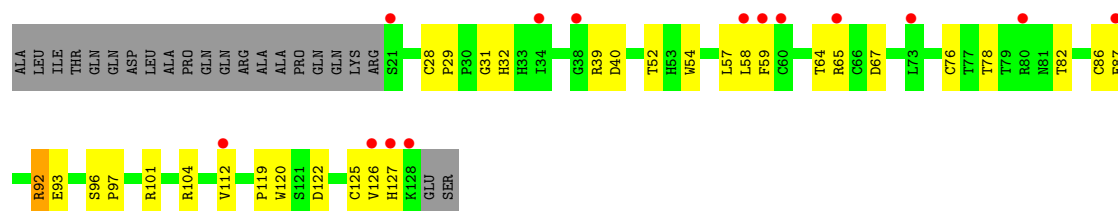
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	R	40	Total 40	O 40	0	0
5	S	39	Total 39	O 39	0	0
5	T	26	Total 26	O 26	0	0
5	A	71	Total 71	O 71	0	0
5	B	58	Total 58	O 58	0	0
5	D	50	Total 50	O 50	0	0

3 Residue-property plots


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. 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. 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.

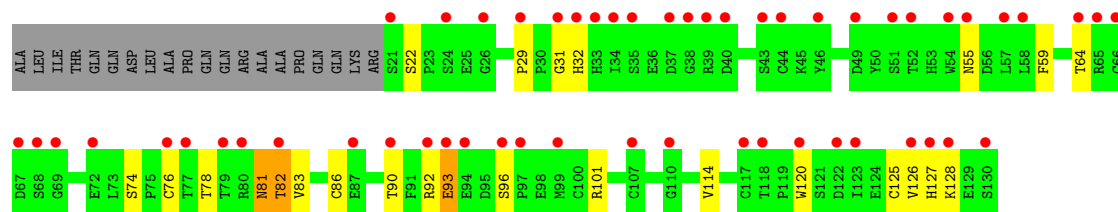
• Molecule 1: DEATH RECEPTOR-5

Chain R: 



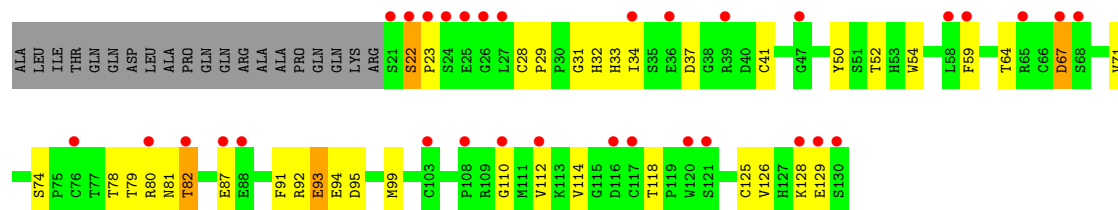
• Molecule 1: DEATH RECEPTOR-5

Chain S: 



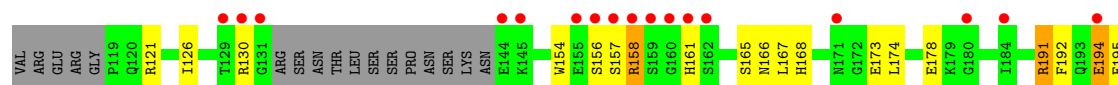
• Molecule 1: DEATH RECEPTOR-5

Chain T: 



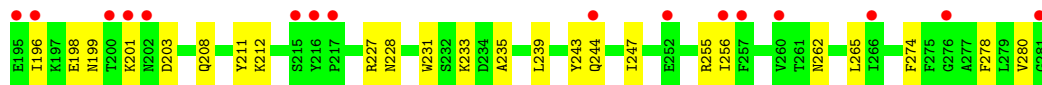
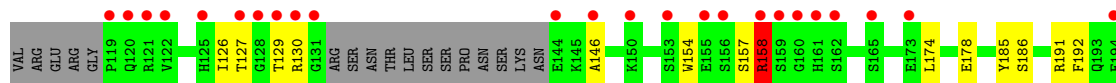
• Molecule 2: APOPTOSIS-2 LIGAND

Chain A: 

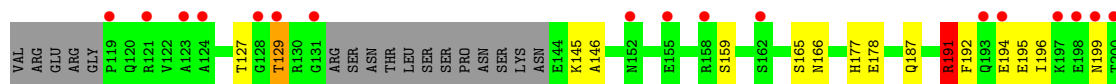




• Molecule 2: APOPTOSIS-2 LIGAND



• Molecule 2: APOPTOSIS-2 LIGAND



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	66.82Å 111.02Å 130.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.40 30.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.3 (30.00-2.40) 99.5 (30.00-2.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.88 (at 2.39Å)	Xtriage
Refinement program	X-PLOR 98.1	Depositor
R, R_{free}	0.222 , 0.267 0.282 , 0.311	Depositor DCC
R_{free} test set	3794 reflections (9.82%)	wwPDB-VP
Wilson B-factor (Å ²)	44.7	Xtriage
Anisotropy	0.458	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 32.1	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	0.89	EDS
Total number of atoms	6576	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% 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: CL, ZN

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	R	0.55	0/851	0.82	0/1150
1	S	0.51	0/867	0.77	0/1170
1	T	0.53	0/867	0.83	1/1170 (0.1%)
2	A	0.85	4/1288 (0.3%)	0.86	2/1729 (0.1%)
2	B	0.68	0/1288	0.90	4/1729 (0.2%)
2	D	0.64	0/1288	0.86	2/1729 (0.1%)
All	All	0.66	4/6449 (0.1%)	0.85	9/8677 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	198	GLU	CG-CD	13.26	1.71	1.51
2	A	198	GLU	CD-OE1	9.97	1.36	1.25
2	A	198	GLU	CD-OE2	6.88	1.33	1.25
2	A	194	GLU	CB-CG	-5.27	1.42	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	158	ARG	NE-CZ-NH2	-9.43	115.59	120.30
2	B	158	ARG	CG-CD-NE	6.93	126.36	111.80
2	B	158	ARG	NE-CZ-NH1	6.85	123.73	120.30
1	T	129	GLU	N-CA-C	-6.62	93.14	111.00
2	D	191	ARG	NE-CZ-NH1	5.57	123.09	120.30
2	D	129	THR	N-CA-C	-5.33	96.62	111.00
2	B	129	THR	N-CA-C	-5.27	96.76	111.00
2	A	198	GLU	N-CA-C	5.20	125.04	111.00
2	A	167	LEU	CA-CB-CG	5.04	126.88	115.30

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	R	833	0	755	25	0
1	S	849	0	766	19	0
1	T	849	0	766	27	0
2	A	1253	0	1204	37	0
2	B	1253	0	1204	34	0
2	D	1253	0	1204	31	0
3	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	71	0	0	3	0
5	B	58	0	0	0	0
5	D	50	0	0	4	0
5	R	40	0	0	0	0
5	S	39	0	0	1	0
5	T	26	0	0	0	0
All	All	6576	0	5899	146	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 12.

All (146) 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:B:158:ARG:N	2:B:158:ARG:HD3	1.75	1.01
2:A:192:PHE:CD1	2:A:194:GLU:HG2	1.97	1.00
2:B:158:ARG:HD3	2:B:158:ARG:H	1.31	0.93
1:R:67:ASP:HB3	2:A:130:ARG:HH12	1.49	0.77
1:T:28:CYS:SG	1:T:34:ILE:HG22	2.26	0.76
2:A:228:ASN:HD22	2:B:239:LEU:H	1.34	0.75
2:B:228:ASN:HD22	2:D:239:LEU:H	1.34	0.75
2:A:239:LEU:H	2:D:228:ASN:HD22	1.35	0.74
1:R:39:ARG:HG2	1:R:39:ARG:HH11	1.55	0.71
2:A:278:PHE:HD2	2:D:247:ILE:HD11	1.57	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:93:GLU:HG2	1:T:94:GLU:N	2.06	0.70
1:S:86:CYS:SG	1:S:92:ARG:HD3	2.31	0.70
2:D:129:THR:HG23	5:D:282:HOH:O	1.90	0.70
1:R:67:ASP:HB3	2:A:130:ARG:NH1	2.07	0.69
1:T:92:ARG:HG3	1:T:92:ARG:HH11	1.60	0.67
1:S:64:THR:H	1:S:81:ASN:HD21	1.40	0.67
1:T:110:GLY:HA2	1:T:128:LYS:HE3	1.76	0.67
1:S:92:ARG:HG2	1:S:96:SER:O	1.95	0.67
1:T:33:HIS:HD2	1:T:34:ILE:O	1.79	0.66
2:B:157:SER:HA	2:B:158:ARG:NH1	2.11	0.66
2:B:247:ILE:HD11	2:D:278:PHE:HD2	1.61	0.66
2:B:158:ARG:H	2:B:158:ARG:CD	2.01	0.66
1:S:76:CYS:HB2	1:S:82:THR:HG22	1.77	0.66
2:A:192:PHE:HD1	2:A:194:GLU:HG2	1.57	0.65
2:A:214:THR:HG23	2:A:215:SER:N	2.13	0.64
1:T:52:THR:HG22	1:T:79:THR:O	1.99	0.62
2:A:208:GLN:HE21	2:A:244:GLN:HE21	1.46	0.62
1:S:64:THR:O	1:S:82:THR:HG21	1.99	0.62
2:B:191:ARG:HG2	2:B:191:ARG:HH11	1.66	0.61
1:R:104:ARG:HD3	1:R:122:ASP:OD2	1.99	0.61
2:B:192:PHE:HB3	2:B:265:LEU:HD22	1.82	0.61
1:T:93:GLU:HG2	1:T:94:GLU:H	1.66	0.60
1:S:74:SER:HB2	1:S:83:VAL:HG23	1.83	0.60
1:R:101:ARG:HB3	2:D:201:LYS:NZ	2.17	0.60
1:T:64:THR:O	1:T:82:THR:HG21	2.03	0.59
2:A:192:PHE:HB3	2:A:265:LEU:HD22	1.84	0.59
2:A:158:ARG:HG2	2:A:161:HIS:HA	1.85	0.59
1:R:76:CYS:HB2	1:R:82:THR:OG1	2.02	0.59
2:A:208:GLN:NE2	2:A:244:GLN:HE21	2.01	0.58
1:T:71:VAL:HG13	1:T:87:GLU:OE1	2.04	0.58
2:D:127:THR:HG22	2:D:274:PHE:HB3	1.85	0.57
1:R:29:PRO:HG2	1:R:32:HIS:CD2	2.39	0.57
1:R:126:VAL:HG22	1:R:127:HIS:H	1.70	0.57
2:A:247:ILE:HD11	2:B:278:PHE:HD2	1.69	0.57
1:T:50:TYR:CZ	1:T:81:ASN:HB2	2.39	0.56
2:B:208:GLN:HE21	2:B:244:GLN:HE21	1.55	0.55
2:D:192:PHE:HB3	2:D:265:LEU:HD22	1.88	0.55
1:S:93:GLU:HG3	1:S:96:SER:OG	2.07	0.55
2:A:191:ARG:HH11	2:A:191:ARG:CG	2.20	0.55
1:T:74:SER:HB2	1:T:80:ARG:HH21	1.71	0.55
2:D:191:ARG:CG	2:D:191:ARG:HH11	2.20	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:59:PHE:CD2	2:D:159:SER:HA	2.42	0.54
2:A:239:LEU:H	2:D:228:ASN:ND2	2.00	0.54
2:A:228:ASN:ND2	2:B:239:LEU:H	2.03	0.54
2:D:146:ALA:HB1	2:D:211:TYR:CE2	2.43	0.54
2:B:278:PHE:CE1	2:B:280:VAL:HG12	2.44	0.53
1:R:101:ARG:HB3	2:D:201:LYS:HZ1	1.74	0.53
2:A:278:PHE:CD2	2:D:247:ILE:HD11	2.42	0.53
1:S:127:HIS:HB3	5:S:144:HOH:O	2.08	0.53
2:B:262:ASN:HB3	2:B:265:LEU:HD12	1.91	0.52
2:A:168:HIS:HB2	5:A:359:HOH:O	2.09	0.52
2:B:247:ILE:HD11	2:D:278:PHE:CD2	2.44	0.52
1:T:33:HIS:CD2	1:T:34:ILE:O	2.62	0.52
2:B:201:LYS:HE3	5:D:330:HOH:O	2.09	0.52
1:R:86:CYS:SG	1:R:92:ARG:HD3	2.50	0.52
1:S:128:LYS:O	1:S:128:LYS:HG3	2.10	0.52
1:R:119:PRO:HG2	1:R:120:TRP:CZ3	2.46	0.51
2:A:227[A]:ARG:NH1	2:B:227[A]:ARG:HH12	2.09	0.50
1:R:31:GLY:HA2	1:R:78:THR:O	2.11	0.50
1:R:39:ARG:HG2	1:R:39:ARG:NH1	2.26	0.50
1:R:67:ASP:CG	2:A:191:ARG:HH22	2.14	0.50
2:D:278:PHE:CE1	2:D:280:VAL:HG12	2.47	0.50
2:B:186:SER:HB3	2:B:208:GLN:NE2	2.28	0.48
2:D:203:ASP:HB3	2:D:231:TRP:CZ3	2.49	0.48
1:R:125:CYS:HB2	2:D:199:ASN:HD21	1.78	0.48
2:D:203:ASP:HA	5:D:297:HOH:O	2.13	0.48
1:T:29:PRO:HG2	1:T:32:HIS:CD2	2.50	0.47
1:S:125:CYS:O	2:A:199:ASN:ND2	2.46	0.47
1:S:59:PHE:CE2	2:B:158:ARG:HB2	2.49	0.47
1:S:74:SER:HB2	1:S:83:VAL:CG2	2.44	0.47
2:D:208:GLN:HE21	2:D:244:GLN:HE21	1.62	0.47
1:R:57:LEU:HB3	1:R:59:PHE:O	2.15	0.46
2:B:146:ALA:HB1	2:B:211:TYR:CE2	2.51	0.46
1:T:22:SER:HA	1:T:23:PRO:HD3	1.75	0.46
2:A:227[A]:ARG:HH12	2:D:227[A]:ARG:NH1	2.13	0.46
1:R:65:ARG:HB3	2:A:130:ARG:HD2	1.99	0.45
2:A:247:ILE:HG13	2:B:185:TYR:OH	2.15	0.45
2:A:270:HIS:HD2	5:A:339:HOH:O	1.99	0.45
2:B:208:GLN:NE2	2:B:244:GLN:HE21	2.14	0.45
2:A:192:PHE:CD1	2:A:194:GLU:CG	2.86	0.45
1:R:126:VAL:HG22	1:R:127:HIS:N	2.32	0.45
1:T:125:CYS:HB2	2:B:199:ASN:OD1	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:55:ASN:HB2	5:A:335:HOH:O	2.17	0.45
1:T:114:VAL:HG21	1:T:126:VAL:HG13	1.99	0.45
2:B:243:TYR:CD1	2:B:243:TYR:C	2.91	0.45
2:D:177:HIS:O	2:D:252:GLU:HG3	2.17	0.45
1:R:39:ARG:HG3	1:R:40:ASP:N	2.32	0.45
1:S:31:GLY:HA2	1:S:78:THR:O	2.18	0.44
2:A:173:GLU:HG2	2:A:257:PHE:HB3	1.99	0.44
1:R:28:CYS:O	1:R:54:TRP:HA	2.18	0.44
1:S:90:THR:HA	1:S:101:ARG:O	2.18	0.44
1:R:96:SER:N	1:R:97:PRO:HD3	2.33	0.44
1:T:23:PRO:HG3	1:T:41:CYS:SG	2.57	0.44
1:T:31:GLY:HA2	1:T:78:THR:O	2.18	0.44
2:A:231:TRP:CD2	2:B:235:ALA:HA	2.53	0.43
1:R:112:VAL:HG13	1:R:126:VAL:HG12	2.00	0.43
2:D:191:ARG:HH11	2:D:191:ARG:HG2	1.82	0.43
2:B:278:PHE:HE1	2:B:280:VAL:HG12	1.82	0.43
1:T:50:TYR:CE2	1:T:81:ASN:HB2	2.53	0.43
1:T:93:GLU:OE2	1:T:95:ASP:HB2	2.18	0.43
1:T:92:ARG:HG3	1:T:92:ARG:NH1	2.29	0.43
2:A:165:SER:O	2:A:166:ASN:HB2	2.18	0.43
2:A:212:LYS:HA	2:A:255:ARG:O	2.19	0.43
1:R:39:ARG:NH1	1:R:39:ARG:CG	2.82	0.43
2:B:212:LYS:HA	2:B:255:ARG:O	2.19	0.43
1:T:67:ASP:CG	2:D:191:ARG:HH22	2.22	0.42
2:B:201:LYS:HE2	2:B:201:LYS:HB3	1.86	0.42
2:D:191:ARG:CG	2:D:191:ARG:NH1	2.82	0.42
1:S:29:PRO:HG2	1:S:32:HIS:CD2	2.54	0.42
1:S:64:THR:O	1:S:82:THR:CG2	2.66	0.42
2:D:187:GLN:HA	2:D:242:ILE:O	2.20	0.42
2:B:127:THR:HG22	2:B:274:PHE:HB3	2.02	0.42
2:B:126:ILE:HD12	2:B:154:TRP:CB	2.50	0.42
1:S:76:CYS:HB2	1:S:82:THR:CG2	2.47	0.41
2:B:158:ARG:N	2:B:158:ARG:CD	2.56	0.41
2:A:174:LEU:HB2	2:A:256:ILE:HG13	2.01	0.41
2:A:126:ILE:HD12	2:A:154:TRP:CB	2.51	0.41
1:R:64:THR:HG22	1:R:65:ARG:N	2.34	0.41
2:B:174:LEU:HB2	2:B:256:ILE:HG13	2.02	0.41
2:D:191:ARG:HG2	2:D:191:ARG:NH1	2.35	0.41
2:D:165:SER:O	2:D:166:ASN:HB2	2.21	0.41
1:T:99:MET:HE2	1:T:99:MET:HB3	1.26	0.41
2:B:203:ASP:HB3	2:B:231:TRP:CZ3	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:191:ARG:CG	2:A:191:ARG:NH1	2.82	0.41
1:S:114:VAL:HG21	1:S:126:VAL:HG22	2.02	0.41
1:T:110:GLY:HA2	1:T:128:LYS:CE	2.48	0.41
1:R:119:PRO:HG2	1:R:120:TRP:CE3	2.56	0.40
2:A:121:ARG:NH2	5:D:318:HOH:O	2.51	0.40
2:A:126:ILE:HD12	2:A:154:TRP:HB3	2.03	0.40
2:D:243:TYR:CD1	2:D:243:TYR:C	2.95	0.40
1:T:91:PHE:HB3	1:T:118:THR:O	2.20	0.40
2:A:231:TRP:CG	2:B:235:ALA:HA	2.56	0.40
1:T:28:CYS:O	1:T:54:TRP:HA	2.21	0.40
2:D:194:GLU:O	2:D:194:GLU:HG3	2.21	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	R	106/130 (82%)	104 (98%)	2 (2%)	0	100	100
1	S	108/130 (83%)	106 (98%)	2 (2%)	0	100	100
1	T	108/130 (83%)	106 (98%)	2 (2%)	0	100	100
2	A	148/168 (88%)	138 (93%)	8 (5%)	2 (1%)	9	13
2	B	148/168 (88%)	140 (95%)	6 (4%)	2 (1%)	9	13
2	D	148/168 (88%)	137 (93%)	10 (7%)	1 (1%)	19	29
All	All	766/894 (86%)	731 (95%)	30 (4%)	5 (1%)	19	29

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	157	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	198	GLU
2	A	198	GLU
2	B	196	ILE
2	D	196	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	R	99/117 (85%)	94 (95%)	5 (5%)	20	35
1	S	101/117 (86%)	96 (95%)	5 (5%)	20	36
1	T	101/117 (86%)	95 (94%)	6 (6%)	16	28
2	A	134/149 (90%)	126 (94%)	8 (6%)	16	27
2	B	134/149 (90%)	130 (97%)	4 (3%)	36	57
2	D	134/149 (90%)	126 (94%)	8 (6%)	16	27
All	All	703/798 (88%)	667 (95%)	36 (5%)	20	35

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	R	52	THR
1	R	58	LEU
1	R	87	GLU
1	R	92	ARG
1	R	93	GLU
1	S	22	SER
1	S	81	ASN
1	S	82	THR
1	S	93	GLU
1	S	120	TRP
1	T	22	SER
1	T	37	ASP
1	T	67	ASP
1	T	82	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	T	93	GLU
1	T	112	VAL
2	A	156	SER
2	A	158	ARG
2	A	178	GLU
2	A	191	ARG
2	A	195	GLU
2	A	196	ILE
2	A	214	THR
2	A	233	LYS
2	B	130	ARG
2	B	158	ARG
2	B	178	GLU
2	B	233	LYS
2	D	145	LYS
2	D	178	GLU
2	D	191	ARG
2	D	195	GLU
2	D	213	TYR
2	D	227[A]	ARG
2	D	227[B]	ARG
2	D	233	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	R	32	HIS
1	R	48	GLN
1	S	32	HIS
1	S	33	HIS
1	S	81	ASN
1	T	32	HIS
1	T	33	HIS
1	T	127	HIS
2	A	208	GLN
2	A	228	ASN
2	A	270	HIS
2	B	208	GLN
2	B	228	ASN
2	B	270	HIS
2	D	208	GLN
2	D	228	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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 ⓘ

Warning: The R factor obtained from EDS is 0.2878, which does not match the depositor's R factor of 0.222. Please interpret the results in this section carefully.

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	R	108/130 (83%)	1.05	14 (12%) 9 7	32, 49, 78, 97	0
1	S	110/130 (84%)	2.12	54 (49%) 0 0	29, 47, 81, 96	0
1	T	110/130 (84%)	1.61	32 (29%) 1 1	34, 48, 84, 97	0
2	A	151/168 (89%)	1.29	27 (17%) 4 4	21, 38, 81, 92	3 (1%)
2	B	151/168 (89%)	1.61	40 (26%) 2 2	21, 34, 74, 98	5 (3%)
2	D	151/168 (89%)	1.05	24 (15%) 6 5	21, 38, 76, 95	5 (3%)
All	All	781/894 (87%)	1.43	191 (24%) 2 2	21, 43, 81, 98	13 (1%)

All (191) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	131	GLY	5.5
2	D	131	GLY	5.5
1	T	130	SER	4.9
1	T	110	GLY	4.9
2	D	198	GLU	4.9
2	D	129	THR	4.8
1	S	126	VAL	4.5
2	A	159	SER	4.5
2	B	129	THR	4.4
2	B	281	GLY	4.3
1	T	24	SER	4.2
2	B	196	ILE	4.2
1	T	34	ILE	4.2
2	A	194	GLU	4.2
2	A	157	SER	4.1
1	S	34	ILE	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	R	34	ILE	4.1
2	A	160	GLY	4.0
2	B	119	PRO	4.0
2	B	195	GLU	4.0
1	S	52	THR	3.9
1	S	66	CYS	3.9
2	B	153	SER	3.9
2	B	156	SER	3.9
2	B	131	GLY	3.8
2	A	196	ILE	3.8
1	S	24	SER	3.7
2	B	159	SER	3.7
1	S	127	HIS	3.7
1	S	39	ARG	3.7
1	S	33	HIS	3.6
1	S	87	GLU	3.6
2	A	218	ASP	3.6
2	B	155	GLU	3.6
1	S	51	SER	3.5
1	S	77	THR	3.5
2	A	161	HIS	3.5
1	T	128	LYS	3.5
1	S	29	PRO	3.4
2	B	202	ASN	3.4
1	T	112	VAL	3.4
1	S	44	CYS	3.4
1	S	68	SER	3.3
1	S	97	PRO	3.3
1	T	120	TRP	3.3
2	A	129	THR	3.3
1	T	22	SER	3.3
2	B	260	VAL	3.2
2	D	193	GLN	3.2
1	S	54	TRP	3.2
2	A	198	GLU	3.2
2	B	194	GLU	3.2
1	S	40	ASP	3.2
2	A	199	ASN	3.2
2	D	199	ASN	3.1
1	T	25	GLU	3.1
1	R	127	HIS	3.1
1	S	130	SER	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	158	ARG	3.1
2	D	194	GLU	3.1
2	A	158	ARG	3.1
2	A	281	GLY	3.1
2	B	266	ILE	3.1
2	A	217	PRO	3.1
1	S	94	GLU	3.0
2	A	180	GLY	3.0
1	S	92	ARG	3.0
1	S	64	THR	3.0
1	S	120	TRP	3.0
1	R	87	GLU	3.0
1	S	35	SER	2.9
2	A	145	LYS	2.9
1	S	93	GLU	2.9
2	A	280	VAL	2.9
1	S	123	ILE	2.9
1	R	73	LEU	2.9
1	S	21	SER	2.9
1	S	46	TYR	2.9
2	A	200	THR	2.9
1	T	59	PHE	2.8
2	B	215	SER	2.8
1	T	27	LEU	2.8
1	S	38	GLY	2.8
2	B	158	ARG	2.8
1	S	31	GLY	2.8
1	S	128	LYS	2.8
1	S	110	GLY	2.8
1	T	39	ARG	2.7
2	B	252	GLU	2.7
2	A	162	SER	2.7
2	B	127	THR	2.7
2	B	200	THR	2.7
2	B	216	TYR	2.7
1	R	80	ARG	2.6
1	S	37	ASP	2.6
1	S	26	GLY	2.6
2	D	281	GLY	2.6
1	S	76	CYS	2.6
1	S	79	THR	2.6
1	T	23	PRO	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	T	108	PRO	2.6
1	S	58	LEU	2.6
1	S	96	SER	2.6
1	S	117	CYS	2.6
2	A	238	GLY	2.6
2	A	227[A]	ARG	2.6
1	R	21	SER	2.6
2	B	122	VAL	2.6
1	S	67	ASP	2.6
1	S	69	GLY	2.6
1	S	118	THR	2.5
1	R	128	LYS	2.5
1	T	26	GLY	2.5
1	R	65	ARG	2.5
1	T	76	CYS	2.5
1	R	126	VAL	2.5
2	B	146	ALA	2.5
1	S	82	THR	2.5
1	S	43	SER	2.5
1	S	65	ARG	2.5
2	D	280	VAL	2.4
2	B	128	GLY	2.4
1	T	65	ARG	2.4
1	T	117	CYS	2.4
2	D	119	PRO	2.4
1	S	57	LEU	2.3
1	T	88	GLU	2.3
2	B	173	GLU	2.3
2	D	128	GLY	2.3
2	D	200	THR	2.3
1	S	32	HIS	2.3
1	S	80	ARG	2.3
2	A	130	ARG	2.3
1	R	38	GLY	2.3
2	B	150	LYS	2.3
2	D	197	LYS	2.3
1	T	36	GLU	2.3
2	B	120	GLN	2.3
1	S	107	CYS	2.3
1	R	59	PHE	2.3
1	T	87	GLU	2.3
2	B	121	ARG	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	A	144	GLU	2.2
2	A	155	GLU	2.2
1	T	103	CYS	2.2
1	T	121	SER	2.2
2	D	152	ASN	2.2
2	D	228	ASN	2.2
1	T	129	GLU	2.2
2	B	244	GLN	2.2
2	B	256	ILE	2.2
1	T	82	THR	2.2
1	T	116	ASP	2.2
2	D	227[A]	ARG	2.2
2	B	217	PRO	2.2
2	D	233	LYS	2.2
1	S	99	MET	2.1
2	B	130	ARG	2.1
1	S	90	THR	2.1
2	B	144	GLU	2.1
2	A	171	ASN	2.1
2	B	125	HIS	2.1
2	D	123	ALA	2.1
2	D	277	ALA	2.1
1	T	47	GLY	2.1
1	T	80	ARG	2.1
2	A	156	SER	2.1
2	D	162	SER	2.1
1	S	49	ASP	2.1
1	R	58	LEU	2.1
1	T	58	LEU	2.1
1	T	21	SER	2.1
2	B	165	SER	2.1
2	D	124	ALA	2.1
2	B	276	GLY	2.1
2	D	278	PHE	2.1
2	D	155	GLU	2.1
1	T	67	ASP	2.1
1	R	112	VAL	2.0
2	D	121	ARG	2.0
2	B	160	GLY	2.0
2	B	201	LYS	2.0
2	B	257	PHE	2.0
1	S	72	GLU	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	162	SER	2.0
1	R	60	CYS	2.0
1	S	122	ASP	2.0
1	T	68	SER	2.0
2	B	161	HIS	2.0
2	A	184	ILE	2.0
1	S	55	ASN	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
3	ZN	A	300	1/1	0.94	0.11	44,44,44,44	0
4	CL	B	400	1/1	0.96	0.06	29,29,29,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.