



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 30, 2014 – 08:29 PM EDT

PDB ID : 4UR3
Title : Crystal structure of the PCE reductive dehalogenase from *S. multivorans* P2(1) crystal form
Authors : Bommer, M.; Kunze, C.; Fessler, J.; Schubert, T.; Diekert, G.; Dobbek, H.
Deposited on : 2014-06-25
Resolution : 2.23 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

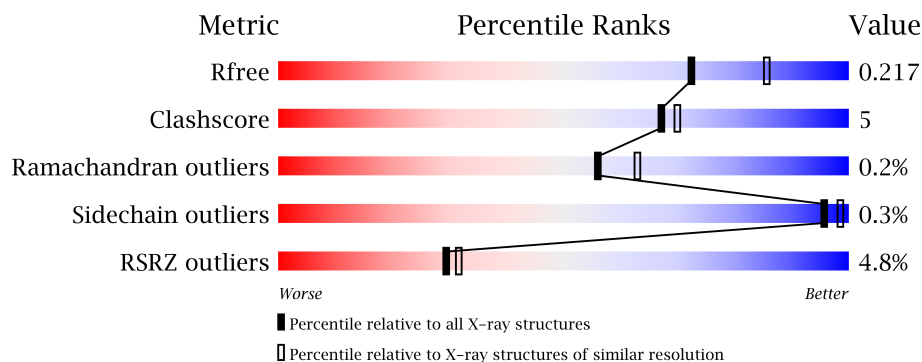
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable24103
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.1.3
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable24103

1 Overall quality at a glance

The reported resolution of this entry is 2.23 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}	66092	1112 (2.26-2.22)
Clashscore	79885	1317 (2.26-2.22)
Ramachandran outliers	78287	1282 (2.26-2.22)
Sidechain outliers	78261	1282 (2.26-2.22)
RSRZ outliers	66119	1112 (2.26-2.22)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	464	
1	B	464	
1	C	464	
1	D	464	
1	E	464	
1	F	464	

2 Entry composition i

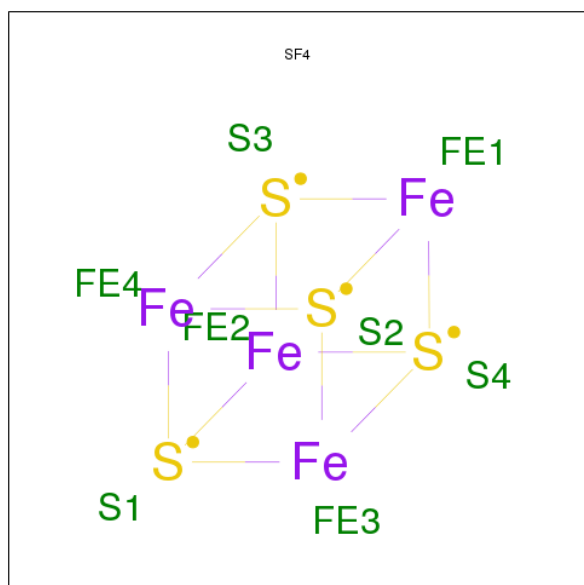
There are 4 unique types of molecules in this entry. The entry contains 22528 atoms, of which 0 are hydrogen and 0 are deuterium.

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 TETRACHLOROETHENE REDUCTIVE DEHALOGENASE CATALYTIC SUBUNIT.

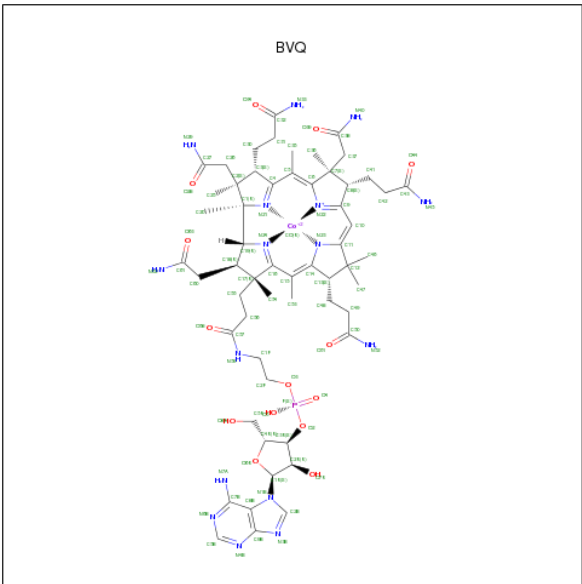
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	458	Total	C	N	O	S	0	0	0
			3608	2291	618	667	32			
1	B	436	Total	C	N	O	S	0	1	0
			3443	2185	588	639	31			
1	C	442	Total	C	N	O	S	0	1	0
			3497	2221	598	647	31			
1	D	437	Total	C	N	O	S	0	0	0
			3444	2186	589	639	30			
1	E	435	Total	C	N	O	S	0	1	0
			3436	2181	587	637	31			
1	F	429	Total	C	N	O	S	0	0	0
			3385	2153	578	624	30			

- Molecule 2 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Fe S 8 4 4	0	0
2	A	1	Total Fe S 8 4 4	0	0
2	B	1	Total Fe S 8 4 4	0	0
2	B	1	Total Fe S 8 4 4	0	0
2	C	1	Total Fe S 8 4 4	0	0
2	C	1	Total Fe S 8 4 4	0	0
2	D	1	Total Fe S 8 4 4	0	0
2	D	1	Total Fe S 8 4 4	0	0
2	E	1	Total Fe S 8 4 4	0	0
2	E	1	Total Fe S 8 4 4	0	0
2	F	1	Total Fe S 8 4 4	0	0
2	F	1	Total Fe S 8 4 4	0	0

- Molecule 3 is NORPSEUDO-B12 (three-letter code: BVQ) (formula: C₅₇H₈₂CoN₁₆O₁₄P).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 89	C 57	Co 1	N 16	O 14	P 1	0	0
3	B	1	Total 89	C 57	Co 1	N 16	O 14	P 1	0	0
3	C	1	Total 89	C 57	Co 1	N 16	O 14	P 1	0	0
3	D	1	Total 89	C 57	Co 1	N 16	O 14	P 1	0	0
3	E	1	Total 89	C 57	Co 1	N 16	O 14	P 1	0	0
3	F	1	Total 89	C 57	Co 1	N 16	O 14	P 1	0	0

- Molecule 4 is water.

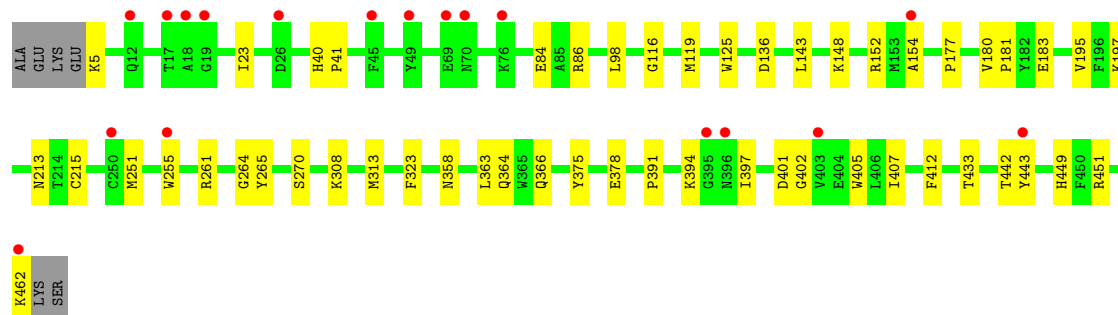
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	193	Total	O	0	0
			193	193		
4	B	204	Total	O	0	0
			204	204		
4	C	254	Total	O	0	0
			254	254		
4	D	199	Total	O	0	0
			199	199		
4	E	103	Total	O	0	0
			103	103		
4	F	132	Total	O	0	0
			132	132		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

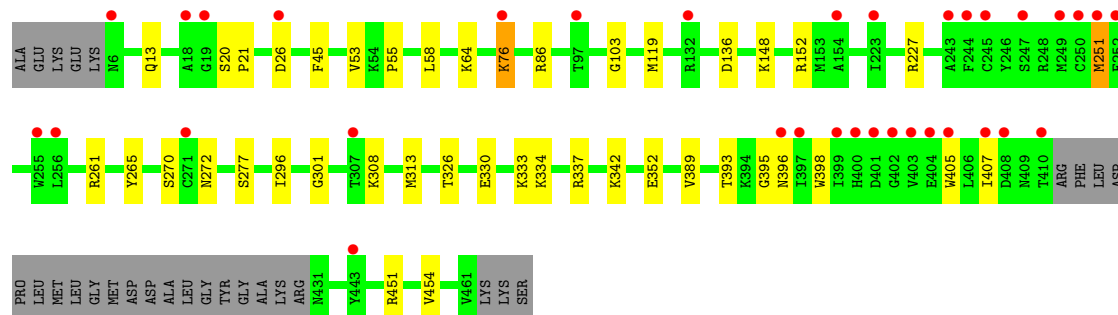
- Molecule 1: TETRACHLOROETHENE REDUCTIVE DEHALOGENASE CATALYTIC SUB-UNIT

Chain A: 



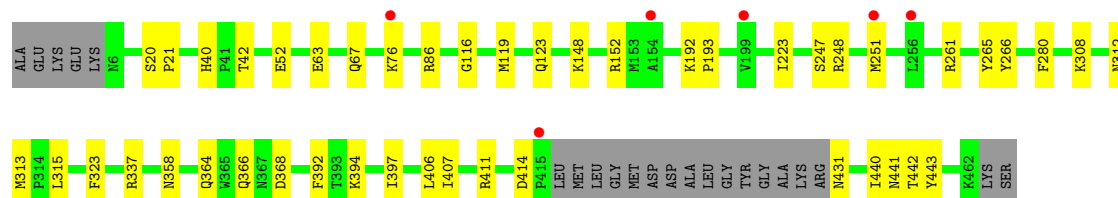
- Molecule 1: TETRACHLOROETHENE REDUCTIVE DEHALOGENASE CATALYTIC SUB-UNIT

Chain B: 



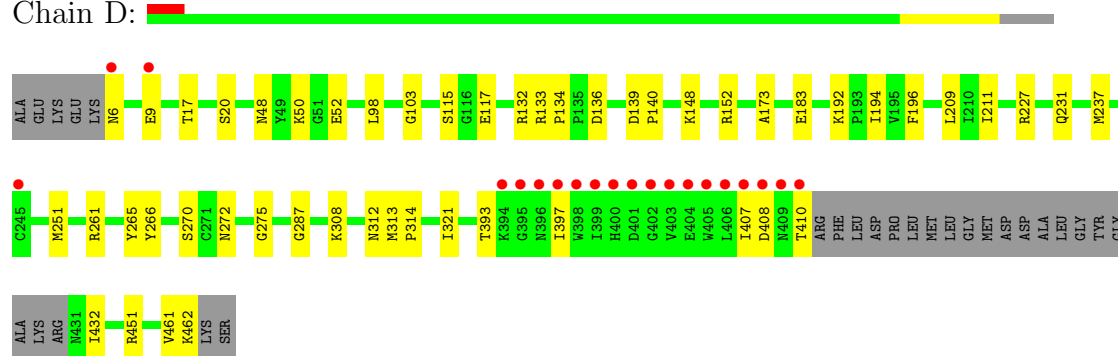
- Molecule 1: TETRACHLOROETHENE REDUCTIVE DEHALOGENASE CATALYTIC SUB-UNIT

Chain C: 



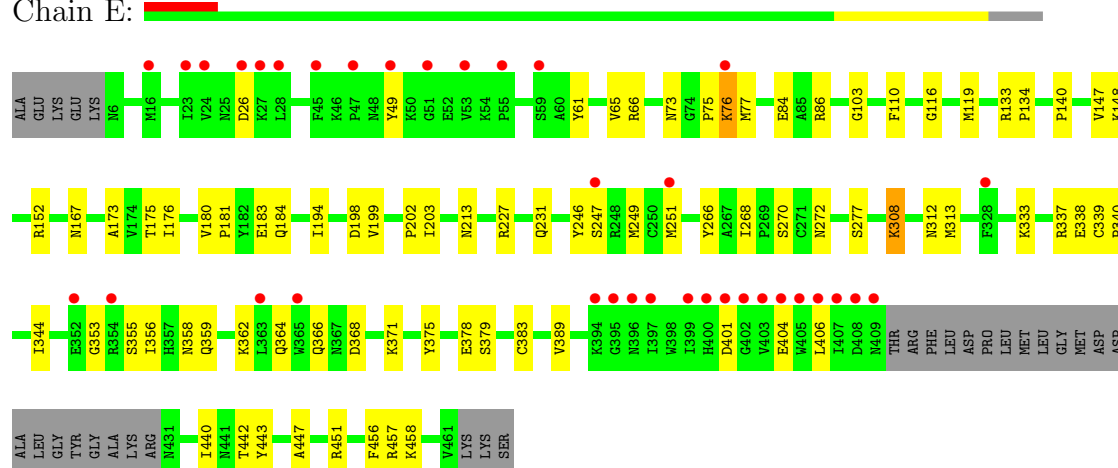
• Molecule 1: TETRACHLOROETHENE REDUCTIVE DEHALOGENASE CATALYTIC SUB-UNIT

Chain D:



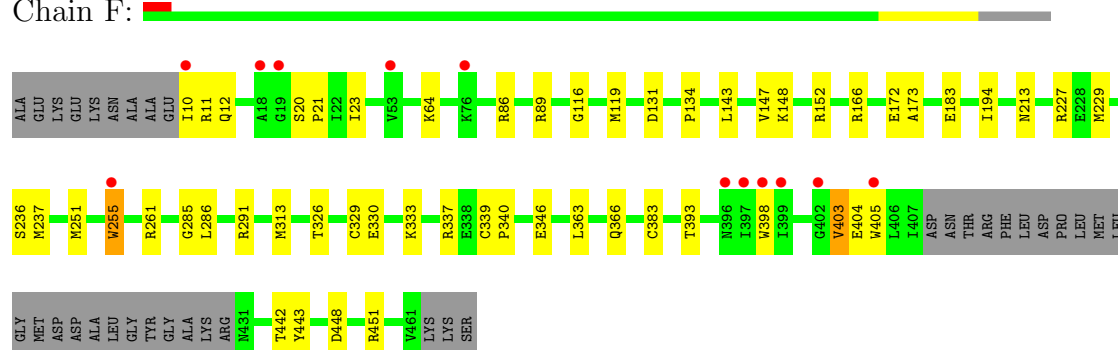
• Molecule 1: TETRACHLOROETHENE REDUCTIVE DEHALOGENASE CATALYTIC SUB-UNIT

Chain E:



• Molecule 1: TETRACHLOROETHENE REDUCTIVE DEHALOGENASE CATALYTIC SUB-UNIT

Chain F:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.31Å 110.60Å 178.79Å 90.00° 95.91° 90.00°	Depositor
Resolution (Å)	48.76 – 2.23 48.76 – 2.24	Depositor EDS
% Data completeness (in resolution range)	98.4 (48.76-2.23) 98.5 (48.76-2.24)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.27 (at 2.24Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.179 , 0.218 0.179 , 0.217	Depositor DCC
R_{free} test set	6849 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	27.7	Xtriage
Anisotropy	0.219	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 35.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	5 of 137023 reflections (0.004%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	22528	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.24	0/3701	0.44	0/5024
1	B	0.28	1/3532 (0.0%)	0.45	0/4798
1	C	0.25	0/3588	0.46	0/4873
1	D	0.27	0/3533	0.47	0/4799
1	E	0.28	0/3525	0.52	2/4788 (0.0%)
1	F	0.24	0/3474	0.46	0/4719
All	All	0.26	1/21353 (0.0%)	0.47	2/29001 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	76	LYS	CE-NZ	6.88	1.66	1.49

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	26	ASP	CB-CG-OD1	6.53	124.17	118.30
1	E	76	LYS	CA-CB-CG	5.32	125.10	113.40

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3608	0	3505	36	0
1	B	3443	0	3329	30	0
1	C	3497	0	3386	33	0
1	D	3444	0	3334	33	0
1	E	3436	0	3322	60	0
1	F	3385	0	3282	41	0
2	A	16	0	0	0	0
2	B	16	0	0	0	0
2	C	16	0	0	0	0
2	D	16	0	0	0	0
2	E	16	0	0	1	0
2	F	16	0	0	1	0
3	A	89	0	0	0	0
3	B	89	0	0	0	0
3	C	89	0	0	0	0
3	D	89	0	0	0	0
3	E	89	0	0	1	0
3	F	89	0	0	0	0
4	A	193	0	0	4	0
4	B	204	0	0	4	0
4	C	254	0	0	3	0
4	D	199	0	0	5	0
4	E	103	0	0	2	0
4	F	132	0	0	4	0
All	All	22528	0	20158	208	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

All (208) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:50:LYS:NZ	4:D:2034:HOH:O	1.94	0.99
1:F:227:ARG:NH1	1:F:393:THR:O	2.02	0.92
1:D:227:ARG:NH1	1:D:393:THR:O	2.10	0.84
1:F:11:ARG:NH2	1:F:285:GLY:O	2.14	0.80
1:E:338:GLU:HG2	1:E:389:VAL:HG11	1.64	0.79
1:E:247:SER:HB2	1:F:255:TRP:CZ2	2.21	0.76
1:D:275:GLY:O	1:D:308:LYS:NZ	2.19	0.75
1:A:364:GLN:HE21	1:A:366:GLN:HE22	1.33	0.73
1:F:89:ARG:HH11	1:F:236:SER:HB3	1.53	0.73
1:F:64:LYS:HG2	1:F:89:ARG:HE	1.54	0.73
1:A:119:MET:SD	4:A:2068:HOH:O	2.47	0.73
1:E:247:SER:HB2	1:F:255:TRP:HZ2	1.52	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:359:GLN:OE1	1:E:362:LYS:NZ	2.21	0.71
1:F:89:ARG:NH1	1:F:236:SER:HB3	2.06	0.71
1:B:119:MET:SD	4:B:2075:HOH:O	2.49	0.70
1:E:358:ASN:HB3	1:E:366:GLN:HE21	1.57	0.69
1:B:313:MET:SD	4:B:2147:HOH:O	2.50	0.68
1:F:64:LYS:NZ	4:F:2027:HOH:O	2.27	0.68
1:D:227:ARG:NH1	4:D:2130:HOH:O	2.26	0.66
1:C:86:ARG:NH1	1:D:134:PRO:O	2.19	0.66
1:E:456:PHE:HB3	1:E:458:LYS:HE2	1.77	0.65
1:E:451:ARG:HD2	1:F:451:ARG:HH21	1.61	0.65
1:F:172:GLU:OE2	4:F:2079:HOH:O	2.14	0.64
1:D:20:SER:O	4:D:2008:HOH:O	2.15	0.64
1:F:143:LEU:HB3	1:F:313:MET:HE3	1.80	0.63
1:F:403:VAL:HG12	1:F:404:GLU:HG3	1.80	0.63
1:E:333:LYS:HB2	1:E:337:ARG:HE	1.64	0.62
1:D:270:SER:OG	1:D:308:LYS:HG3	2.00	0.61
1:E:451:ARG:NH2	1:F:448:ASP:OD1	2.34	0.61
1:B:334:LYS:HD3	1:B:389:VAL:HB	1.83	0.60
1:C:358:ASN:HB3	1:C:366:GLN:HE21	1.65	0.60
1:E:355:SER:OG	1:E:356:ILE:N	2.33	0.60
1:A:364:GLN:HE21	1:A:366:GLN:NE2	1.98	0.59
1:E:173:ALA:HB2	1:E:194:ILE:HD11	1.84	0.59
1:C:364:GLN:HE21	1:C:366:GLN:NE2	2.00	0.59
1:B:227:ARG:NH1	1:B:393:THR:O	2.35	0.59
1:E:458:LYS:H	1:E:458:LYS:HD3	1.68	0.59
1:E:86:ARG:NH1	1:F:134:PRO:O	2.34	0.59
1:A:270:SER:OG	1:A:308:LYS:HG3	2.03	0.58
1:E:198:ASP:OD1	1:E:213:ASN:ND2	2.36	0.58
1:C:251[A]:MET:SD	1:D:251:MET:HG3	2.44	0.58
1:E:451:ARG:HD2	1:F:451:ARG:NH2	2.18	0.57
1:D:132:ARG:NH2	4:D:2082:HOH:O	2.37	0.57
1:C:431:ASN:N	4:C:2234:HOH:O	2.37	0.57
1:C:392:PHE:HA	1:C:397:ILE:HD12	1.87	0.56
1:E:458:LYS:N	1:E:458:LYS:HD3	2.19	0.56
1:E:75:PRO:O	1:E:76:LYS:HB2	2.05	0.56
1:F:291:ARG:NH1	1:F:329:CYS:O	2.39	0.56
1:F:346:GLU:O	4:F:2117:HOH:O	2.18	0.55
1:D:17:THR:HG23	1:E:140:PRO:HG3	1.89	0.54
1:E:75:PRO:HG3	1:E:379:SER:HA	1.89	0.54
1:D:397:ILE:HG12	1:D:407:ILE:HG23	1.87	0.54
1:A:375:TYR:HA	1:A:378:GLU:HG3	1.90	0.54
1:E:76:LYS:HB3	1:E:77:MET:HG2	1.90	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:401:ASP:OD2	1:E:404:GLU:HG2	2.08	0.53
1:A:264:GLY:HA2	4:A:2077:HOH:O	2.09	0.53
1:C:86:ARG:HD2	1:D:136:ASP:OD2	2.09	0.53
1:A:98:LEU:CD2	1:A:251:MET:HG2	2.39	0.53
1:E:251[A]:MET:SD	1:F:251:MET:HG3	2.49	0.53
1:F:366:GLN:NE2	4:F:2120:HOH:O	2.31	0.53
1:C:313:MET:HE2	1:C:315:LEU:HD21	1.91	0.53
1:C:364:GLN:HE21	1:C:366:GLN:HE22	1.57	0.53
1:B:333:LYS:HB2	1:B:337:ARG:HH11	1.73	0.53
1:C:76:LYS:O	1:C:76:LYS:HG3	2.07	0.53
1:A:116:GLY:HA2	1:A:119:MET:HE3	1.90	0.52
1:E:202:PRO:HB3	1:E:268:ILE:HD11	1.91	0.52
1:E:375:TYR:HA	1:E:378:GLU:HG3	1.91	0.52
1:F:23:ILE:HD11	1:F:363:LEU:HD22	1.92	0.51
1:B:26:ASP:OD1	4:B:2016:HOH:O	2.19	0.51
1:D:287:GLY:HA2	1:D:321:ILE:HD11	1.92	0.51
1:A:213:ASN:ND2	4:A:2105:HOH:O	2.33	0.51
1:B:333:LYS:HB2	1:B:337:ARG:NH1	2.26	0.51
1:E:457:ARG:HB3	4:E:2096:HOH:O	2.10	0.51
1:E:75:PRO:HD3	1:E:379:SER:O	2.11	0.51
1:C:63:GLU:O	1:C:67:GLN:HG3	2.11	0.51
1:E:61:TYR:O	1:E:65:VAL:HG23	2.10	0.50
1:A:397:ILE:HD11	1:A:412:PHE:CZ	2.46	0.50
1:F:147:VAL:HB	1:F:313:MET:HE2	1.92	0.50
1:D:173:ALA:HB2	1:D:194:ILE:HD11	1.93	0.50
1:C:86:ARG:NH2	1:D:133:ARG:O	2.36	0.50
1:E:277:SER:OG	1:E:308:LYS:NZ	2.44	0.50
1:C:52:GLU:OE1	4:C:2040:HOH:O	2.20	0.49
1:B:270:SER:OG	1:B:308:LYS:HG3	2.11	0.49
1:D:231:GLN:NE2	4:D:2131:HOH:O	2.45	0.49
1:D:6:ASN:HB3	1:D:9:GLU:OE1	2.13	0.49
1:A:401:ASP:OD1	1:A:402:GLY:N	2.45	0.49
1:E:227:ARG:O	1:E:231:GLN:HG2	2.12	0.49
1:E:266:TYR:CZ	1:E:312:ASN:HB3	2.48	0.49
1:B:13:GLN:OE1	1:B:405:TRP:HB2	2.12	0.49
1:C:368:ASP:OD2	4:C:2222:HOH:O	2.20	0.49
1:A:391:PRO:HA	1:A:394:LYS:HG2	1.94	0.49
1:E:368:ASP:OD1	1:E:371:LYS:HG2	2.14	0.48
1:E:199:VAL:HG21	1:E:203:ILE:HD13	1.94	0.48
1:A:323:PHE:HD2	1:A:407:ILE:HD11	1.78	0.48
1:E:451:ARG:NH2	1:F:448:ASP:HA	2.29	0.48
1:E:246:TYR:O	1:E:249:MET:HB2	2.14	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:154:ALA:HA	1:A:255:TRP:CE3	2.49	0.47
1:F:166:ARG:NH2	1:F:213:ASN:OD1	2.44	0.47
1:C:261:ARG:HA	1:C:265:TYR:O	2.14	0.47
1:C:337:ARG:NH2	1:C:414:ASP:OD2	2.48	0.47
1:E:353:GLY:HA2	1:E:366:GLN:HG2	1.97	0.47
1:A:358:ASN:HB3	1:A:366:GLN:HE21	1.79	0.47
1:E:333:LYS:HG3	1:E:337:ARG:HH21	1.79	0.47
1:E:383:CYS:HB3	2:E:502:SF4:S1	2.53	0.47
1:A:451:ARG:HH22	1:B:451:ARG:HH12	1.61	0.47
1:B:148:LYS:O	1:B:152:ARG:HG2	2.14	0.47
1:A:5:LYS:HA	1:A:405:TRP:CH2	2.50	0.46
1:E:364:GLN:HE22	3:E:503:BVQ:P	2.38	0.46
1:F:333:LYS:HB2	1:F:337:ARG:NH1	2.30	0.46
1:E:442:THR:HG22	1:E:443:TYR:CD2	2.50	0.46
1:A:23:ILE:HD11	1:A:363:LEU:HD23	1.97	0.46
1:B:277:SER:OG	1:B:308:LYS:HE3	2.15	0.46
1:F:119:MET:HE1	1:F:261:ARG:NH1	2.31	0.46
1:E:451:ARG:NH1	1:F:451:ARG:HH22	2.13	0.46
1:B:261:ARG:HA	1:B:265:TYR:O	2.15	0.46
1:E:270:SER:OG	1:E:308:LYS:HG3	2.16	0.46
1:F:229:MET:HB3	1:F:237:MET:O	2.16	0.46
1:A:397:ILE:HD11	1:A:412:PHE:CE1	2.50	0.46
1:E:180:VAL:HA	1:E:181:PRO:HD3	1.62	0.46
1:F:383:CYS:HB3	2:F:502:SF4:S1	2.56	0.46
1:E:406:LEU:HD23	1:E:406:LEU:HA	1.57	0.46
1:E:183:GLU:H	1:E:183:GLU:CD	2.18	0.45
1:F:11:ARG:HH22	1:F:286:LEU:HA	1.82	0.45
1:D:115:SER:OG	1:D:117:GLU:HG3	2.16	0.45
1:E:447:ALA:HB1	1:F:451:ARG:HG3	1.99	0.45
1:A:261:ARG:HA	1:A:265:TYR:O	2.16	0.45
1:B:45:PHE:HD2	1:B:53:VAL:HG12	1.81	0.45
1:A:86:ARG:NH1	1:B:136:ASP:OD2	2.46	0.45
1:A:181:PRO:HB2	1:A:183:GLU:OE2	2.16	0.45
1:A:449:HIS:ND1	4:A:2188:HOH:O	2.36	0.45
1:C:116:GLY:HA2	1:C:119:MET:HE3	1.98	0.45
1:C:148:LYS:O	1:C:152:ARG:HG2	2.16	0.45
1:A:251:MET:HE2	1:B:251[B]:MET:SD	2.56	0.44
1:A:136:ASP:OD2	1:B:86:ARG:HD2	2.18	0.44
1:A:195:VAL:HG21	1:A:197:LYS:HE3	1.99	0.44
1:D:261:ARG:HA	1:D:265:TYR:O	2.18	0.44
1:C:247:SER:HB3	1:D:251:MET:HE1	1.99	0.44
1:C:119:MET:HE3	1:C:261:ARG:NH1	2.32	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:326:THR:O	1:F:330:GLU:HG3	2.17	0.44
1:D:139:ASP:HA	1:D:140:PRO:HD2	1.83	0.44
1:E:344:ILE:O	4:E:2083:HOH:O	2.21	0.44
1:F:116:GLY:HA2	1:F:119:MET:CE	2.48	0.44
1:C:20:SER:HA	1:C:21:PRO:HD3	1.73	0.44
1:B:352:GLU:OE2	4:B:2018:HOH:O	2.21	0.44
1:B:398:TRP:CZ3	1:B:407:ILE:HG13	2.53	0.44
1:B:55:PRO:HD2	1:B:58:LEU:HD12	2.00	0.44
1:C:323:PHE:HD2	1:C:407:ILE:HD11	1.82	0.44
1:C:280:PHE:CD2	1:C:308:LYS:HD2	2.53	0.43
1:E:147:VAL:HG21	1:E:313:MET:HE3	2.00	0.43
1:C:440:ILE:HG13	1:C:441:ASN:N	2.33	0.43
1:E:133:ARG:HA	1:E:134:PRO:HD3	1.90	0.43
1:F:339:CYS:HA	1:F:340:PRO:HD3	1.78	0.43
1:F:398:TRP:HB3	1:F:405:TRP:CE3	2.53	0.43
1:B:342:LYS:HD3	1:B:342:LYS:HA	1.72	0.43
1:C:116:GLY:HA2	1:C:119:MET:CE	2.48	0.43
1:A:462:LYS:HE2	1:A:462:LYS:HB2	1.57	0.43
1:A:451:ARG:HH22	1:B:451:ARG:NH1	2.16	0.43
1:B:326:THR:O	1:B:330:GLU:HG3	2.18	0.43
1:C:266:TYR:CZ	1:C:312:ASN:HB3	2.54	0.43
1:D:237:MET:HG2	1:D:432:ILE:HD13	2.01	0.43
1:B:103:GLY:O	1:B:272:ASN:HB2	2.19	0.43
1:C:223:ILE:HG23	1:C:248:ARG:CZ	2.49	0.43
1:D:313:MET:HA	1:D:314:PRO:HD3	1.91	0.43
1:E:181:PRO:HD2	1:E:184:GLN:OE1	2.19	0.43
1:C:123:GLN:OE1	1:D:183:GLU:HG3	2.19	0.43
1:D:148:LYS:O	1:D:152:ARG:HG2	2.19	0.43
1:F:131:ASP:OD1	1:F:131:ASP:N	2.52	0.43
1:F:173:ALA:HB2	1:F:194:ILE:HD11	2.01	0.43
1:B:451:ARG:O	1:B:454:VAL:HG12	2.18	0.42
1:A:125:TRP:CH2	1:B:64:LYS:HE2	2.54	0.42
1:F:442:THR:HG22	1:F:443:TYR:CD2	2.54	0.42
1:D:48:ASN:OD1	1:D:52:GLU:HG3	2.19	0.42
1:E:75:PRO:O	1:E:76:LYS:CB	2.67	0.42
1:C:442:THR:HG22	1:C:443:TYR:CD2	2.55	0.42
1:D:266:TYR:CZ	1:D:312:ASN:HB3	2.54	0.42
1:A:442:THR:HG22	1:A:443:TYR:CD2	2.55	0.42
1:E:73:ASN:ND2	1:E:84:GLU:OE2	2.43	0.42
1:D:103:GLY:O	1:D:272:ASN:HB2	2.19	0.42
1:E:49:TYR:CE2	1:E:66:ARG:HD3	2.55	0.42
1:E:175:THR:OG1	1:E:176:ILE:N	2.53	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:98:LEU:CD2	1:D:251:MET:HG2	2.50	0.41
1:B:227:ARG:NH2	1:B:395:GLY:HA3	2.35	0.41
1:E:339:CYS:HA	1:E:340:PRO:HD3	1.78	0.41
1:E:103:GLY:O	1:E:272:ASN:HB2	2.20	0.41
1:D:196:PHE:HA	1:D:211:ILE:O	2.21	0.41
1:E:148:LYS:O	1:E:152:ARG:HG2	2.21	0.41
1:F:148:LYS:O	1:F:152:ARG:HG2	2.20	0.41
1:A:148:LYS:O	1:A:152:ARG:HG2	2.20	0.41
1:D:408:ASP:CG	1:D:410:THR:HB	2.41	0.41
1:F:10:ILE:HG23	1:F:12:GLN:H	1.84	0.41
1:C:394:LYS:NZ	1:C:411:ARG:O	2.51	0.41
1:E:133:ARG:HG2	1:F:86:ARG:HH12	1.85	0.41
1:A:451:ARG:NH2	1:B:451:ARG:HH12	2.19	0.41
1:D:192:LYS:HD2	1:D:209:LEU:HG	2.03	0.41
1:C:76:LYS:O	1:C:76:LYS:CG	2.69	0.41
1:A:143:LEU:HD13	1:A:313:MET:HG3	2.02	0.41
1:A:177:PRO:HG2	1:A:180:VAL:CG2	2.51	0.40
1:B:296:ILE:HG23	1:B:301:GLY:HA2	2.03	0.40
1:E:199:VAL:HG21	1:E:203:ILE:CD1	2.51	0.40
1:C:40:HIS:CE1	1:C:42:THR:HG1	2.38	0.40
1:D:461:VAL:C	1:D:462:LYS:HD2	2.41	0.40
1:E:440:ILE:HA	1:E:440:ILE:HD12	1.88	0.40
1:F:20:SER:HA	1:F:21:PRO:HD2	1.93	0.40
1:A:40:HIS:CD2	1:A:41:PRO:HD2	2.56	0.40
1:A:84:GLU:OE1	1:A:433:THR:OG1	2.21	0.40
1:C:192:LYS:HA	1:C:193:PRO:HD3	1.92	0.40
1:B:20:SER:HA	1:B:21:PRO:HD3	1.75	0.40
1:E:116:GLY:HA2	1:E:119:MET:CE	2.52	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	456/464 (98%)	443 (97%)	12 (3%)	1 (0%)	56	63
1	B	433/464 (93%)	415 (96%)	16 (4%)	2 (0%)	38	37
1	C	439/464 (95%)	426 (97%)	13 (3%)	0	100	100
1	D	433/464 (93%)	421 (97%)	12 (3%)	0	100	100
1	E	432/464 (93%)	411 (95%)	20 (5%)	1 (0%)	56	63
1	F	425/464 (92%)	412 (97%)	12 (3%)	1 (0%)	56	63
All	All	2618/2784 (94%)	2528 (97%)	85 (3%)	5 (0%)	56	63

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	76	LYS
1	B	396	ASN
1	F	403	VAL
1	A	215	CYS
1	E	110	PHE

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	384/389 (99%)	384 (100%)	0	100	100
1	B	368/389 (95%)	366 (100%)	2 (0%)	94	97
1	C	374/389 (96%)	373 (100%)	1 (0%)	96	98
1	D	368/389 (95%)	367 (100%)	1 (0%)	96	98
1	E	367/389 (94%)	365 (100%)	2 (0%)	94	97
1	F	362/389 (93%)	360 (99%)	2 (1%)	92	96
All	All	2223/2334 (95%)	2215 (100%)	8 (0%)	96	98

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	251[A]	MET
1	B	251[B]	MET

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Mol	Chain	Res	Type
1	C	406	LEU
1	D	451	ARG
1	E	167	ASN
1	E	308	LYS
1	F	183	GLU
1	F	255	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	366	GLN
1	C	366	GLN
1	D	231	GLN
1	E	167	ASN
1	E	366	GLN
1	E	370	ASN
1	E	409	ASN
1	E	449	HIS

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

18 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
2	SF4	A	501	1	12,12,12	10.35	10 (83%)	0,24,24	0.00	-
2	SF4	A	502	1	12,12,12	11.87	12 (100%)	0,24,24	0.00	-
3	BVQ	A	503	4	99,99,99	0.84	5 (5%)	147,162,162	1.31	19 (12%)
2	SF4	B	501	1	12,12,12	10.62	12 (100%)	0,24,24	0.00	-
2	SF4	B	502	1	12,12,12	10.62	12 (100%)	0,24,24	0.00	-
3	BVQ	B	503	4	99,99,99	0.85	5 (5%)	147,162,162	1.47	21 (14%)
2	SF4	C	501	1	12,12,12	10.65	10 (83%)	0,24,24	0.00	-
2	SF4	C	502	1	12,12,12	13.04	12 (100%)	0,24,24	0.00	-
3	BVQ	C	503	-	99,99,99	0.85	5 (5%)	147,162,162	1.42	20 (13%)
2	SF4	D	501	1	12,12,12	11.66	12 (100%)	0,24,24	0.00	-
2	SF4	D	502	1	12,12,12	10.71	12 (100%)	0,24,24	0.00	-
3	BVQ	D	503	4	99,99,99	0.84	5 (5%)	147,162,162	1.39	23 (15%)
2	SF4	E	501	1	12,12,12	10.22	10 (83%)	0,24,24	0.00	-
2	SF4	E	502	1	12,12,12	12.08	12 (100%)	0,24,24	0.00	-
3	BVQ	E	503	4	99,99,99	0.87	5 (5%)	147,162,162	1.40	23 (15%)
2	SF4	F	501	1	12,12,12	11.34	9 (75%)	0,24,24	0.00	-
2	SF4	F	502	1	12,12,12	11.18	12 (100%)	0,24,24	0.00	-
3	BVQ	F	503	-	99,99,99	0.84	5 (5%)	147,162,162	1.34	19 (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
2	SF4	A	501	1	-	0/0/48/48	0/6/5/5
2	SF4	A	502	1	-	0/0/48/48	0/6/5/5
3	BVQ	A	503	4	-	0/54/221/221	0/3/11/11
2	SF4	B	501	1	-	0/0/48/48	0/6/5/5
2	SF4	B	502	1	-	0/0/48/48	0/6/5/5
3	BVQ	B	503	4	-	0/54/221/221	0/3/11/11
2	SF4	C	501	1	-	0/0/48/48	0/6/5/5
2	SF4	C	502	1	-	0/0/48/48	0/6/5/5
3	BVQ	C	503	-	-	0/54/221/221	0/3/11/11
2	SF4	D	501	1	-	0/0/48/48	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SF4	D	502	1	-	0/0/48/48	0/6/5/5
3	BVQ	D	503	4	-	0/54/221/221	0/3/11/11
2	SF4	E	501	1	-	0/0/48/48	0/6/5/5
2	SF4	E	502	1	-	0/0/48/48	0/6/5/5
3	BVQ	E	503	4	-	0/54/221/221	0/3/11/11
2	SF4	F	501	1	-	0/0/48/48	0/6/5/5
2	SF4	F	502	1	-	0/0/48/48	0/6/5/5
3	BVQ	F	503	-	-	0/54/221/221	0/3/11/11

All (165) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	SF4	S2-FE1	-20.96	2.19	2.33
2	C	501	SF4	S2-FE1	-20.39	2.19	2.33
2	A	502	SF4	S2-FE1	-20.38	2.19	2.33
2	F	501	SF4	S2-FE1	-19.53	2.20	2.33
2	E	501	SF4	S2-FE1	-19.36	2.20	2.33
2	C	502	SF4	S2-FE1	-19.14	2.20	2.33
2	D	501	SF4	S2-FE1	-18.59	2.20	2.33
2	B	502	SF4	S3-FE4	-18.04	2.21	2.33
2	F	502	SF4	S2-FE4	-17.88	2.21	2.33
2	F	501	SF4	S4-FE3	-17.77	2.21	2.33
2	C	502	SF4	S1-FE3	-17.07	2.21	2.33
2	B	501	SF4	S4-FE3	-16.92	2.21	2.33
2	D	501	SF4	S2-FE3	-16.06	2.22	2.33
2	C	502	SF4	S4-FE3	-15.83	2.22	2.33
2	C	501	SF4	S2-FE3	-15.68	2.22	2.33
2	C	502	SF4	S2-FE3	-15.52	2.22	2.33
2	F	502	SF4	S2-FE3	-15.46	2.22	2.33
2	C	502	SF4	S1-FE2	-15.45	2.22	2.33
2	F	501	SF4	S2-FE3	-15.43	2.22	2.33
2	E	502	SF4	S2-FE3	-15.37	2.22	2.33
2	E	502	SF4	S2-FE1	-15.34	2.22	2.33
2	B	502	SF4	S1-FE2	-15.31	2.23	2.33
2	B	501	SF4	S2-FE3	-15.18	2.23	2.33
2	A	502	SF4	S1-FE2	-15.14	2.23	2.33
2	E	502	SF4	S1-FE3	-15.12	2.23	2.33
2	E	501	SF4	S2-FE3	-15.08	2.23	2.33
2	E	502	SF4	S1-FE2	-15.07	2.23	2.33
2	C	501	SF4	S1-FE2	-14.98	2.23	2.33
2	A	501	SF4	S2-FE3	-14.92	2.23	2.33
2	A	502	SF4	S2-FE3	-14.92	2.23	2.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	502	SF4	S2-FE3	-14.92	2.23	2.33
2	B	502	SF4	S2-FE3	-14.87	2.23	2.33
2	D	502	SF4	S1-FE2	-14.87	2.23	2.33
2	F	502	SF4	S1-FE2	-14.76	2.23	2.33
2	E	501	SF4	S1-FE2	-14.72	2.23	2.33
2	D	501	SF4	S1-FE2	-14.60	2.23	2.33
2	F	501	SF4	S1-FE2	-14.57	2.23	2.33
2	D	502	SF4	S2-FE1	-14.48	2.23	2.33
2	A	501	SF4	S1-FE2	-14.29	2.23	2.33
2	F	502	SF4	S1-FE4	-14.28	2.23	2.33
2	B	501	SF4	S1-FE2	-14.27	2.23	2.33
2	D	502	SF4	S4-FE3	-14.07	2.23	2.33
2	E	502	SF4	S1-FE4	-13.33	2.24	2.33
2	A	502	SF4	S1-FE3	-12.97	2.24	2.33
2	A	502	SF4	S1-FE4	-12.81	2.24	2.33
2	B	501	SF4	S1-FE4	-12.74	2.24	2.33
2	B	502	SF4	S2-FE1	-12.39	2.24	2.33
2	C	502	SF4	S2-FE4	-12.33	2.25	2.33
2	D	501	SF4	S3-FE1	-12.25	2.25	2.33
2	F	501	SF4	S4-FE1	-11.75	2.25	2.33
2	D	501	SF4	S4-FE1	-11.72	2.25	2.33
2	A	501	SF4	S4-FE3	-11.56	2.25	2.33
2	B	501	SF4	S4-FE1	-11.52	2.25	2.33
2	E	501	SF4	S4-FE1	-11.20	2.25	2.33
2	A	501	SF4	S4-FE1	-11.16	2.25	2.33
2	C	501	SF4	S4-FE1	-11.13	2.25	2.33
2	D	502	SF4	S4-FE1	-11.08	2.25	2.33
2	E	502	SF4	S4-FE1	-11.06	2.25	2.33
2	D	501	SF4	S4-FE3	-11.05	2.25	2.33
2	A	502	SF4	S4-FE1	-10.97	2.25	2.33
2	F	502	SF4	S4-FE1	-10.89	2.25	2.33
2	E	502	SF4	S2-FE4	-10.68	2.26	2.33
2	D	501	SF4	S1-FE4	-10.58	2.26	2.33
2	B	502	SF4	S4-FE1	-10.58	2.26	2.33
2	C	501	SF4	S3-FE4	-10.53	2.26	2.33
2	C	502	SF4	S1-FE4	-10.42	2.26	2.33
2	E	502	SF4	S4-FE3	-10.42	2.26	2.33
2	C	502	SF4	S4-FE1	-10.37	2.26	2.33
2	D	501	SF4	S3-FE2	-10.29	2.26	2.33
2	D	502	SF4	S1-FE4	-10.27	2.26	2.33
2	B	501	SF4	S3-FE2	-10.24	2.26	2.33
2	F	502	SF4	S4-FE2	-10.14	2.26	2.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	502	SF4	S2-FE4	-9.99	2.26	2.33
2	F	501	SF4	S3-FE2	-9.96	2.26	2.33
2	D	502	SF4	S3-FE2	-9.83	2.26	2.33
2	B	502	SF4	S3-FE2	-9.82	2.26	2.33
2	C	501	SF4	S3-FE2	-9.79	2.26	2.33
2	E	502	SF4	S3-FE2	-9.77	2.26	2.33
2	A	501	SF4	S3-FE2	-9.65	2.26	2.33
2	E	501	SF4	S3-FE2	-9.63	2.26	2.33
2	D	502	SF4	S1-FE3	-9.59	2.26	2.33
2	D	501	SF4	S3-FE4	-9.57	2.26	2.33
2	F	502	SF4	S3-FE2	-9.54	2.26	2.33
2	C	502	SF4	S3-FE2	-9.50	2.26	2.33
2	A	502	SF4	S3-FE2	-9.43	2.26	2.33
2	F	501	SF4	S3-FE4	-9.37	2.26	2.33
2	A	502	SF4	S4-FE3	-9.31	2.27	2.33
2	B	501	SF4	S2-FE4	-8.89	2.27	2.33
2	C	502	SF4	S4-FE2	-8.88	2.27	2.33
2	E	502	SF4	S3-FE4	-8.82	2.27	2.33
2	E	502	SF4	S3-FE1	-8.75	2.27	2.33
2	C	502	SF4	S3-FE1	-8.59	2.27	2.33
2	C	501	SF4	S4-FE3	-8.39	2.27	2.33
2	F	502	SF4	S3-FE4	-8.18	2.27	2.33
2	B	501	SF4	S3-FE1	-8.11	2.27	2.33
2	A	502	SF4	S3-FE1	-7.85	2.28	2.33
2	E	501	SF4	S4-FE3	-7.73	2.28	2.33
2	A	502	SF4	S2-FE4	-7.65	2.28	2.33
2	F	502	SF4	S2-FE1	-7.41	2.28	2.33
2	A	502	SF4	S4-FE2	-7.17	2.28	2.33
2	E	501	SF4	S1-FE4	-7.16	2.28	2.33
2	E	502	SF4	S4-FE2	-7.16	2.28	2.33
2	F	502	SF4	S1-FE3	-6.97	2.28	2.33
2	E	501	SF4	S3-FE1	-6.89	2.28	2.33
2	D	501	SF4	S2-FE4	-6.84	2.28	2.33
2	C	502	SF4	S3-FE4	-6.48	2.28	2.33
2	B	502	SF4	S4-FE3	-6.41	2.28	2.33
2	B	501	SF4	S3-FE4	-6.36	2.29	2.33
2	D	501	SF4	S1-FE3	-6.22	2.29	2.33
2	D	502	SF4	S3-FE4	-6.22	2.29	2.33
2	F	501	SF4	S1-FE4	-6.11	2.29	2.33
2	E	501	SF4	S3-FE4	-5.90	2.29	2.33
2	C	501	SF4	S1-FE3	-5.78	2.29	2.33
2	D	502	SF4	S2-FE4	-5.64	2.29	2.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	502	SF4	S3-FE1	-5.57	2.29	2.33
2	F	501	SF4	S2-FE4	-5.54	2.29	2.33
2	B	501	SF4	S2-FE1	-5.40	2.29	2.33
2	C	501	SF4	S1-FE4	-5.25	2.29	2.33
2	A	501	SF4	S1-FE4	-5.05	2.29	2.33
2	A	502	SF4	S3-FE4	-4.88	2.30	2.33
2	F	502	SF4	S3-FE1	-4.65	2.30	2.33
2	B	502	SF4	S3-FE1	-4.46	2.30	2.33
2	B	502	SF4	S1-FE4	-4.42	2.30	2.33
2	E	501	SF4	S1-FE3	-4.33	2.30	2.33
2	B	502	SF4	S4-FE2	-4.20	2.30	2.33
2	A	501	SF4	S2-FE4	-4.19	2.30	2.33
2	A	501	SF4	S3-FE4	-4.12	2.30	2.33
2	F	502	SF4	S4-FE3	-3.89	2.30	2.33
2	B	502	SF4	S1-FE3	-3.51	2.30	2.33
3	C	503	BVQ	C16-C15	3.36	1.52	1.40
3	A	503	BVQ	C13-C14	3.35	1.59	1.52
3	F	503	BVQ	C16-C15	3.35	1.52	1.40
2	B	501	SF4	S1-FE3	-3.34	2.31	2.33
3	B	503	BVQ	C16-C15	3.29	1.52	1.40
3	E	503	BVQ	C16-C15	3.26	1.52	1.40
3	E	503	BVQ	C13-C14	3.24	1.58	1.52
3	A	503	BVQ	C16-C15	3.18	1.51	1.40
2	D	501	SF4	S4-FE2	-3.17	2.31	2.33
3	D	503	BVQ	C13-C14	3.13	1.58	1.52
3	B	503	BVQ	C13-C14	3.09	1.58	1.52
2	C	501	SF4	S3-FE1	-2.99	2.31	2.33
3	F	503	BVQ	C13-C14	2.98	1.58	1.52
3	E	503	BVQ	C4-C5	2.96	1.50	1.40
3	C	503	BVQ	C13-C14	2.94	1.58	1.52
3	D	503	BVQ	C2B-N1B	-2.92	1.32	1.36
3	E	503	BVQ	C2B-N1B	-2.91	1.32	1.36
3	D	503	BVQ	C16-C15	2.90	1.50	1.40
3	C	503	BVQ	C4-C5	2.88	1.50	1.40
3	C	503	BVQ	C2B-N1B	-2.86	1.32	1.36
2	B	501	SF4	S4-FE2	2.84	2.35	2.33
3	B	503	BVQ	C4-C5	2.83	1.50	1.40
3	F	503	BVQ	C4-C5	2.83	1.50	1.40
3	F	503	BVQ	C2B-N1B	-2.83	1.32	1.36
3	A	503	BVQ	C2B-N1B	-2.78	1.32	1.36
3	B	503	BVQ	C1-N21	-2.76	1.45	1.49
3	D	503	BVQ	C4-C5	2.74	1.50	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	503	BVQ	C2B-N1B	-2.71	1.32	1.36
3	D	503	BVQ	C1-N21	-2.65	1.46	1.49
3	A	503	BVQ	C1-N21	-2.61	1.46	1.49
3	A	503	BVQ	C4-C5	2.54	1.49	1.40
2	A	501	SF4	S4-FE2	2.48	2.34	2.33
3	C	503	BVQ	C1-N21	-2.46	1.46	1.49
3	F	503	BVQ	C1-N21	-2.43	1.46	1.49
2	D	502	SF4	S4-FE2	-2.43	2.31	2.33
3	E	503	BVQ	C1-N21	-2.31	1.46	1.49

All (125) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	503	BVQ	C1R-N1B-C8B	7.16	138.00	125.57
3	C	503	BVQ	C1R-N1B-C8B	6.64	137.10	125.57
3	A	503	BVQ	C35-C5-C6	5.77	127.16	118.75
3	D	503	BVQ	C35-C5-C6	5.52	126.79	118.75
3	D	503	BVQ	C1R-N1B-C8B	5.50	135.11	125.57
3	B	503	BVQ	C35-C5-C6	5.42	126.66	118.75
3	F	503	BVQ	C35-C5-C6	5.35	126.56	118.75
3	C	503	BVQ	C35-C5-C6	5.28	126.45	118.75
3	E	503	BVQ	C35-C5-C6	5.19	126.31	118.75
3	A	503	BVQ	C35-C5-C4	-4.95	111.53	118.75
3	C	503	BVQ	C35-C5-C4	-4.82	111.71	118.75
3	F	503	BVQ	C35-C5-C4	-4.81	111.74	118.75
3	D	503	BVQ	C35-C5-C4	-4.74	111.83	118.75
3	E	503	BVQ	C35-C5-C4	-4.59	112.06	118.75
3	F	503	BVQ	C2B-N1B-C8B	-4.58	103.38	106.83
3	B	503	BVQ	C35-C5-C4	-4.58	112.07	118.75
3	C	503	BVQ	C2B-N1B-C8B	-4.44	103.48	106.83
3	E	503	BVQ	C2B-N1B-C8B	-4.41	103.51	106.83
3	D	503	BVQ	C2B-N1B-C8B	-4.38	103.53	106.83
3	B	503	BVQ	C2B-N1B-C1R	-4.37	117.92	126.15
3	B	503	BVQ	C2B-N1B-C8B	-4.17	103.69	106.83
3	A	503	BVQ	C2B-N1B-C8B	-4.11	103.74	106.83
3	E	503	BVQ	C1R-N1B-C8B	3.86	132.27	125.57
3	E	503	BVQ	C30-C3-C2	-3.82	111.25	119.00
3	C	503	BVQ	C2B-N1B-C1R	-3.63	119.32	126.15
3	A	503	BVQ	C1R-N1B-C8B	3.55	131.72	125.57
3	B	503	BVQ	C8B-C9B-N3B	-3.50	105.63	109.33
3	E	503	BVQ	C2-C1-N21	3.30	104.86	101.51
3	E	503	BVQ	C8B-C9B-N3B	-3.27	105.88	109.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	503	BVQ	C2-C1-N21	3.26	104.82	101.51
3	E	503	BVQ	C9-C10-C11	-3.25	123.99	132.41
3	F	503	BVQ	C9-C10-C11	-3.24	124.00	132.41
3	C	503	BVQ	C9-C10-C11	-3.22	124.05	132.41
3	F	503	BVQ	C30-C3-C2	-3.22	112.46	119.00
3	C	503	BVQ	C2-C1-N21	3.21	104.77	101.51
3	D	503	BVQ	C8B-C9B-N3B	-3.20	105.95	109.33
3	E	503	BVQ	C55-C17-C18	-3.18	104.46	110.98
3	A	503	BVQ	C9-C10-C11	-3.18	124.16	132.41
3	C	503	BVQ	C8B-C9B-N3B	-3.17	105.99	109.33
3	A	503	BVQ	C8B-C9B-N3B	-3.16	105.99	109.33
3	B	503	BVQ	C9-C10-C11	-3.14	124.26	132.41
3	F	503	BVQ	C8B-C9B-N3B	-3.09	106.07	109.33
3	B	503	BVQ	C55-C17-C16	3.06	120.17	110.77
3	D	503	BVQ	C9-C10-C11	-3.06	124.48	132.41
3	C	503	BVQ	C30-C3-C2	-3.02	112.87	119.00
3	E	503	BVQ	C48-C13-C14	2.93	118.70	111.53
3	E	503	BVQ	C8-C9-C10	-2.92	118.20	124.62
3	D	503	BVQ	C2-C1-N21	2.85	104.40	101.51
3	A	503	BVQ	C30-C3-C2	-2.84	113.23	119.00
3	B	503	BVQ	C20-C1-C19	-2.80	106.67	109.40
3	F	503	BVQ	C8-C9-C10	-2.79	118.48	124.62
3	D	503	BVQ	C55-C17-C16	2.79	119.32	110.77
3	E	503	BVQ	C56-C55-C17	-2.74	109.61	115.52
3	A	503	BVQ	C2-C1-N21	2.73	104.28	101.51
3	D	503	BVQ	C2B-N1B-C1R	-2.73	121.02	126.15
3	C	503	BVQ	C8-C9-C10	-2.69	118.70	124.62
3	B	503	BVQ	C30-C3-C2	-2.68	113.55	119.00
3	F	503	BVQ	C55-C17-C16	2.67	118.97	110.77
3	B	503	BVQ	C8-C9-C10	-2.64	118.82	124.62
3	A	503	BVQ	C48-C13-C14	2.64	117.99	111.53
3	D	503	BVQ	C30-C3-C2	-2.62	113.69	119.00
3	F	503	BVQ	C55-C17-C18	-2.54	105.76	110.98
3	A	503	BVQ	C55-C17-C16	2.54	118.56	110.77
3	D	503	BVQ	C48-C13-C14	2.51	117.69	111.53
3	D	503	BVQ	C55-C17-C18	-2.50	105.86	110.98
3	F	503	BVQ	C10-C9-N22	2.47	129.59	123.58
3	C	503	BVQ	C10-C9-N22	2.46	129.57	123.58
3	E	503	BVQ	C55-C17-C16	2.45	118.30	110.77
3	F	503	BVQ	C1R-N1B-C8B	2.45	129.82	125.57
3	D	503	BVQ	C36-C7-C8	-2.43	107.58	112.14
3	B	503	BVQ	C10-C9-N22	2.43	129.50	123.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	503	BVQ	C5-C6-N22	-2.42	120.26	125.01
3	C	503	BVQ	P-O2-C3R	2.38	128.53	119.12
3	D	503	BVQ	C10-C9-N22	2.38	129.38	123.58
3	C	503	BVQ	C55-C17-C16	2.37	118.04	110.77
3	E	503	BVQ	C10-C9-N22	2.35	129.31	123.58
3	C	503	BVQ	C48-C13-C14	2.34	117.27	111.53
3	B	503	BVQ	C2-C1-N21	2.34	103.89	101.51
3	B	503	BVQ	C48-C13-C14	2.34	117.25	111.53
3	C	503	BVQ	C13-C14-C15	-2.30	122.97	131.85
3	D	503	BVQ	C5-C6-N22	-2.30	120.50	125.01
3	C	503	BVQ	C5-C6-N22	-2.29	120.51	125.01
3	E	503	BVQ	O3-P-O2	-2.28	98.19	104.68
3	A	503	BVQ	C20-C1-C19	-2.27	107.18	109.40
3	A	503	BVQ	C5-C6-N22	-2.26	120.58	125.01
3	F	503	BVQ	C13-C14-C15	-2.26	123.17	131.85
3	A	503	BVQ	P-O2-C3R	2.23	127.91	119.12
3	D	503	BVQ	C13-C14-C15	-2.22	123.32	131.85
3	E	503	BVQ	C3-C4-C5	-2.21	123.33	131.85
3	F	503	BVQ	C48-C13-C14	2.21	116.94	111.53
3	C	503	BVQ	C3-C4-C5	-2.21	123.34	131.85
3	D	503	BVQ	C3-C4-C5	-2.21	123.36	131.85
3	F	503	BVQ	C3-C4-C5	-2.20	123.36	131.85
3	F	503	BVQ	C20-C1-C19	-2.20	107.25	109.40
3	B	503	BVQ	C13-C14-C15	-2.20	123.37	131.85
3	D	503	BVQ	P-O2-C3R	2.19	127.78	119.12
3	F	503	BVQ	C5-C6-N22	-2.19	120.72	125.01
3	A	503	BVQ	C10-C9-N22	2.16	128.85	123.58
3	E	503	BVQ	P-O2-C3R	2.16	127.63	119.12
3	A	503	BVQ	C55-C17-C18	-2.15	106.57	110.98
3	E	503	BVQ	C7-C6-C5	2.15	130.84	124.81
3	A	503	BVQ	C3-C4-C5	-2.14	123.61	131.85
3	C	503	BVQ	C3-C4-N21	2.12	113.81	111.06
3	E	503	BVQ	C53-C15-C14	2.12	121.84	118.75
3	B	503	BVQ	C3-C4-C5	-2.12	123.70	131.85
3	A	503	BVQ	C13-C14-C15	-2.11	123.72	131.85
3	D	503	BVQ	C20-C1-C19	-2.11	107.34	109.40
3	E	503	BVQ	C48-C13-C12	-2.10	110.28	116.65
3	B	503	BVQ	C12-C11-N23	2.10	115.29	110.81
3	E	503	BVQ	C13-C14-C15	-2.09	123.81	131.85
3	C	503	BVQ	C7-C6-C5	2.08	130.65	124.81
3	D	503	BVQ	C12-C11-N23	2.08	115.25	110.81
3	D	503	BVQ	C1-C19-C18	-2.07	118.18	121.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	503	BVQ	C12-C11-N23	2.07	115.24	110.81
3	B	503	BVQ	C19-C1-N21	2.07	104.25	102.15
3	C	503	BVQ	C12-C11-N23	2.06	115.22	110.81
3	F	503	BVQ	P-O2-C3R	2.06	127.26	119.12
3	D	503	BVQ	C53-C15-C14	2.06	121.75	118.75
3	B	503	BVQ	P-O2-C3R	2.05	127.22	119.12
3	F	503	BVQ	O3-P-O2	-2.05	98.84	104.68
3	B	503	BVQ	C5-C6-N22	-2.03	121.03	125.01
3	B	503	BVQ	C55-C17-C18	-2.02	106.83	110.98
3	D	503	BVQ	C7-C6-C5	2.01	130.47	124.81
3	E	503	BVQ	C41-C8-C7	2.01	119.87	114.15
3	A	503	BVQ	C36-C7-C8	-2.00	108.38	112.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	458/464 (98%)	0.10	18 (3%)	37 41	20, 35, 53, 67	0
1	B	436/464 (93%)	0.18	34 (7%)	13 15	18, 29, 53, 87	0
1	C	442/464 (95%)	-0.13	6 (1%)	72 76	14, 25, 43, 73	0
1	D	437/464 (94%)	0.04	20 (4%)	31 34	14, 26, 56, 94	0
1	E	435/464 (93%)	0.43	36 (8%)	11 13	22, 46, 67, 85	0
1	F	429/464 (92%)	-0.03	12 (2%)	50 55	21, 38, 61, 77	0
All	All	2637/2784 (94%)	0.10	126 (4%)	29 31	14, 33, 59, 94	0

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	410	THR	8.4
1	B	403	VAL	7.4
1	D	403	VAL	7.0
1	D	407	ILE	6.6
1	E	396	ASN	6.4
1	D	405	TRP	6.3
1	E	403	VAL	6.1
1	D	399	ILE	5.9
1	E	408	ASP	5.7
1	D	396	ASN	5.4
1	F	396	ASN	5.4
1	B	407	ILE	5.4
1	D	398	TRP	5.3
1	F	397	ILE	5.2
1	E	395	GLY	5.1
1	E	26	ASP	5.0
1	B	251[A]	MET	5.0
1	D	401	ASP	4.9
1	D	409	ASN	4.6

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Mol	Chain	Res	Type	RSRZ
1	D	395	GLY	4.5
1	B	402	GLY	4.4
1	B	404	GLU	4.4
1	E	402	GLY	4.3
1	E	399	ILE	4.3
1	F	405	TRP	4.3
1	D	6	ASN	4.3
1	B	400	HIS	4.0
1	B	401	ASP	4.0
1	D	397	ILE	3.9
1	E	401	ASP	3.8
1	D	400	HIS	3.8
1	E	397	ILE	3.8
1	B	399	ILE	3.7
1	E	76	LYS	3.7
1	D	406	LEU	3.7
1	D	402	GLY	3.6
1	E	28	LEU	3.6
1	B	410	THR	3.5
1	E	24	VAL	3.5
1	D	404	GLU	3.5
1	F	19	GLY	3.5
1	E	406	LEU	3.4
1	F	398	TRP	3.4
1	A	18	ALA	3.3
1	E	53	VAL	3.3
1	A	403	VAL	3.3
1	F	18	ALA	3.1
1	B	250	CYS	3.1
1	E	365	TRP	3.1
1	F	76	LYS	3.1
1	D	408	ASP	3.1
1	F	10	ILE	3.0
1	B	249	MET	3.0
1	E	51	GLY	3.0
1	F	402	GLY	3.0
1	A	70	ASN	3.0
1	B	6	ASN	3.0
1	D	394	LYS	2.9
1	F	255	TRP	2.8
1	E	409	ASN	2.8
1	C	251[A]	MET	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	76	LYS	2.8
1	E	394	LYS	2.8
1	A	69	GLU	2.7
1	F	399	ILE	2.7
1	B	443	TYR	2.7
1	E	23	ILE	2.7
1	E	328	PHE	2.7
1	B	26	ASP	2.6
1	B	408	ASP	2.6
1	A	154	ALA	2.6
1	D	9	GLU	2.6
1	B	223	ILE	2.6
1	B	76	LYS	2.5
1	E	59	SER	2.5
1	B	19	GLY	2.5
1	A	26	ASP	2.5
1	B	244	PHE	2.5
1	E	405	TRP	2.5
1	B	396	ASN	2.5
1	B	18	ALA	2.5
1	C	415	PRO	2.4
1	B	255	TRP	2.4
1	E	55	PRO	2.4
1	E	352	GLU	2.4
1	A	396	ASN	2.4
1	B	307	THR	2.4
1	B	405	TRP	2.4
1	E	16	MET	2.4
1	A	76	LYS	2.3
1	A	19	GLY	2.3
1	A	45	PHE	2.3
1	B	243	ALA	2.3
1	B	245	CYS	2.3
1	B	247	SER	2.3
1	E	404	GLU	2.3
1	B	97	THR	2.3
1	E	363	LEU	2.3
1	A	443	TYR	2.2
1	E	247	SER	2.2
1	A	395	GLY	2.2
1	E	407	ILE	2.2
1	A	462	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	252	PHE	2.2
1	F	53	VAL	2.2
1	B	271	CYS	2.2
1	C	256	LEU	2.2
1	B	397	ILE	2.1
1	E	47	PRO	2.1
1	A	250	CYS	2.1
1	D	245	CYS	2.1
1	B	132	ARG	2.1
1	A	255	TRP	2.1
1	E	400	HIS	2.1
1	B	256	LEU	2.1
1	E	354	ARG	2.1
1	A	12	GLN	2.1
1	C	199	VAL	2.1
1	A	49	TYR	2.1
1	E	49	TYR	2.1
1	C	154	ALA	2.1
1	E	251[A]	MET	2.0
1	A	17	THR	2.0
1	B	154	ALA	2.0
1	E	27	LYS	2.0
1	E	45	PHE	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	BVQ	C	503	89/89	0.13	0.24	13,21,28,32	0
2	SF4	C	502	8/8	0.10	0.22	19,23,24,25	0
3	BVQ	B	503	89/89	0.14	0.10	12,22,27,30	0
3	BVQ	D	503	89/89	0.12	-0.13	14,21,26,36	0
3	BVQ	F	503	89/89	0.11	-0.17	19,29,36,50	0
2	SF4	D	502	8/8	0.09	-0.22	22,24,26,29	0
3	BVQ	E	503	89/89	0.13	-0.35	29,42,49,59	0
3	BVQ	A	503	89/89	0.10	-0.47	21,30,36,38	0
2	SF4	C	501	8/8	0.09	-0.68	19,23,25,28	0
2	SF4	B	501	8/8	0.08	-1.09	20,24,25,28	0
2	SF4	A	501	8/8	0.07	-1.42	28,32,34,38	0
2	SF4	F	501	8/8	0.07	-1.49	33,38,41,44	0
2	SF4	E	501	8/8	0.07	-1.53	43,51,52,53	0
2	SF4	B	502	8/8	0.06	-1.57	20,23,24,24	0
2	SF4	D	501	8/8	0.05	-1.66	19,26,28,30	0
2	SF4	A	502	8/8	0.06	-1.82	29,32,35,36	0
2	SF4	F	502	8/8	0.08	-1.83	32,35,39,39	0
2	SF4	E	502	8/8	0.07	-2.12	38,47,52,54	0

6.5 Other polymers ⓘ

There are no such residues in this entry.