



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:04 PM GMT

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 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

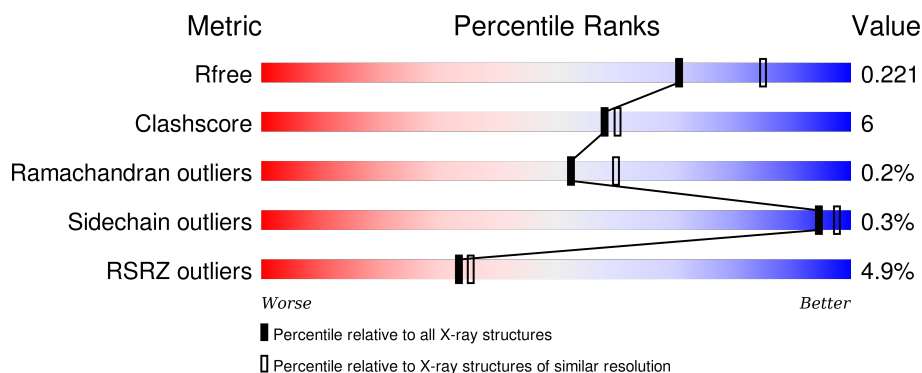
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.23 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}	91344	1611 (2.26-2.22)
Clashscore	102246	1764 (2.26-2.22)
Ramachandran outliers	100387	1724 (2.26-2.22)
Sidechain outliers	100360	1724 (2.26-2.22)
RSRZ outliers	91569	1616 (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. 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	464	<div> <div>4%</div> <div>87% 11% .</div> </div>
1	B	464	<div> <div>8%</div> <div>84% 9% 6%</div> </div>
1	C	464	<div> <div>%</div> <div>85% 11% 5%</div> </div>
1	D	464	<div> <div>4%</div> <div>83% 11% 6%</div> </div>
1	E	464	<div> <div>8%</div> <div>76% 17% 6%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	464	

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
3	BVQ	A	503	X	-	-	-
3	BVQ	B	503	X	-	-	-
3	BVQ	C	503	X	-	-	-
3	BVQ	D	503	X	-	-	-
3	BVQ	E	503	X	-	-	-
3	BVQ	F	503	X	-	-	-

2 Entry composition [i](#)

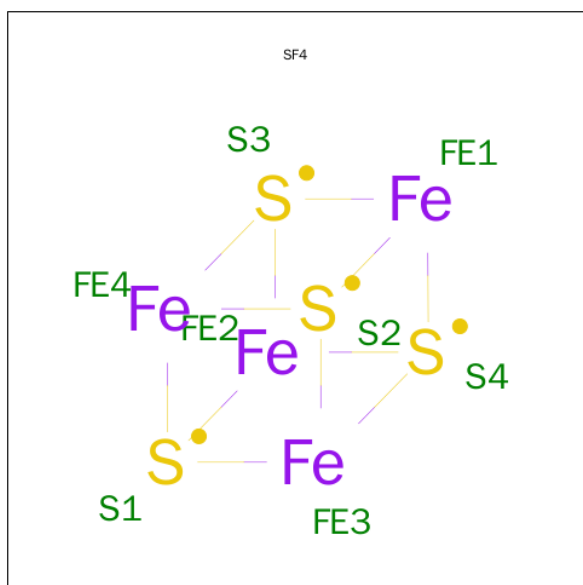
There are 4 unique types of molecules in this entry. The entry contains 22528 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 TETRACHLOROETHENE REDUCTIVE DEHALOGENASE CATALYTIC SUBUNIT.

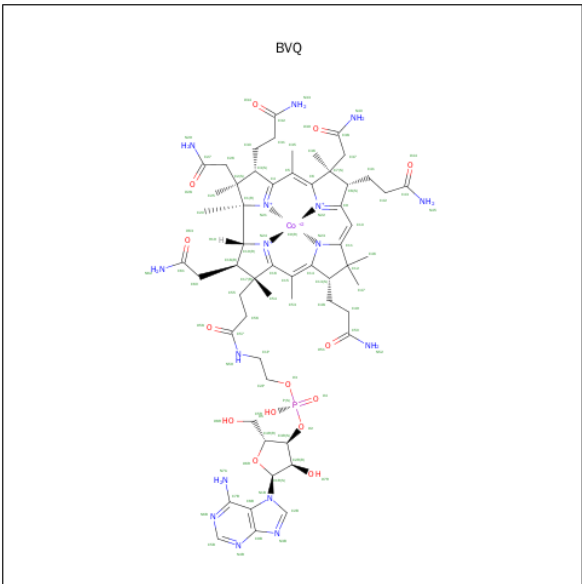
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	458	Total	C	N	O	S	0	0	0
			3608	2291	618	667	32			
1	B	436	Total	C	N	O	S	0	1	0
			3443	2185	588	639	31			
1	C	442	Total	C	N	O	S	0	1	0
			3497	2221	598	647	31			
1	D	437	Total	C	N	O	S	0	0	0
			3444	2186	589	639	30			
1	E	435	Total	C	N	O	S	0	1	0
			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	0	0
			8	4	4		
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2	C	1	Total	Fe	S	0	0
			8	4	4		
2	C	1	Total	Fe	S	0	0
			8	4	4		
2	D	1	Total	Fe	S	0	0
			8	4	4		
2	D	1	Total	Fe	S	0	0
			8	4	4		
2	E	1	Total	Fe	S	0	0
			8	4	4		
2	E	1	Total	Fe	S	0	0
			8	4	4		
2	F	1	Total	Fe	S	0	0
			8	4	4		
2	F	1	Total	Fe	S	0	0
			8	4	4		

- 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

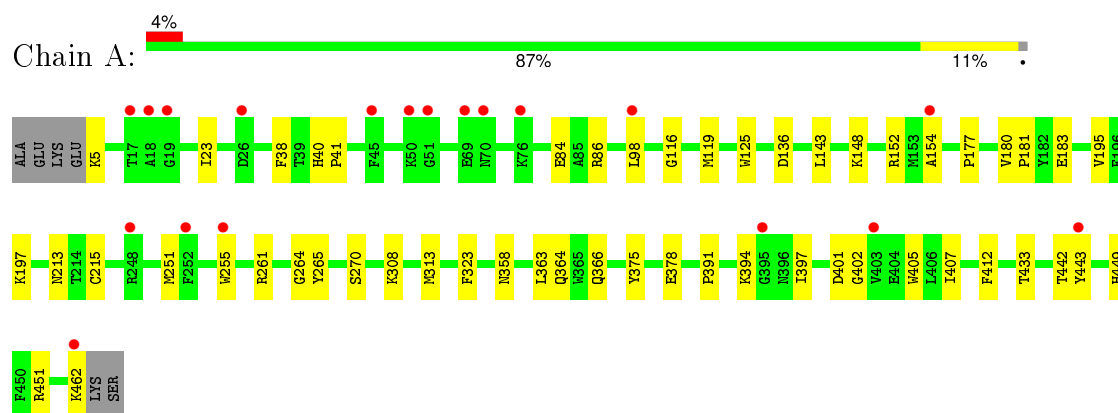
- Molecule 4 is water.

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		

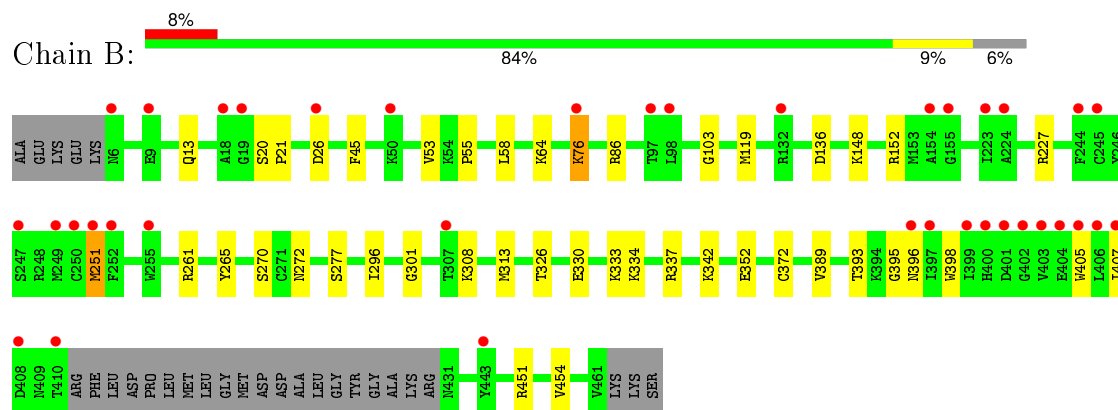
3 Residue-property plots

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.

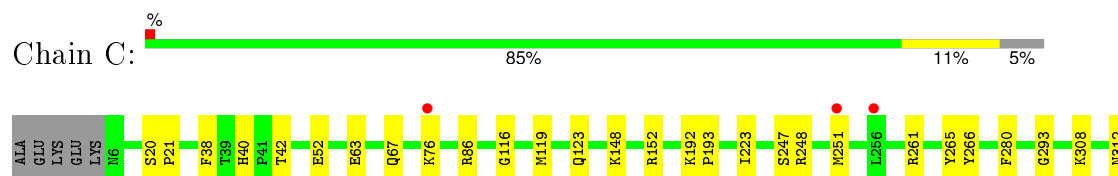
• Molecule 1: TETRACHLOROETHENE REDUCTIVE DEHALOGENASE CATALYTIC SUB-UNIT



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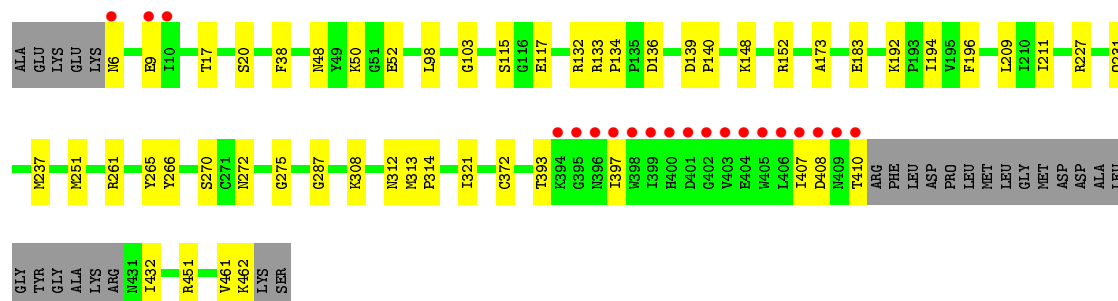
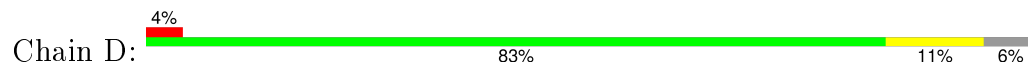


• Molecule 1: TETRACHLOROETHENE REDUCTIVE DEHALOGENASE CATALYTIC SUB-UNIT

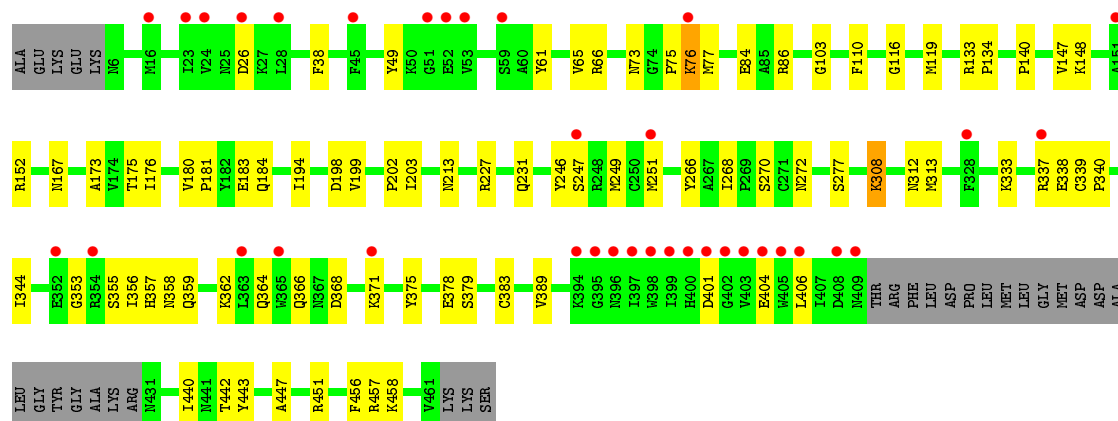
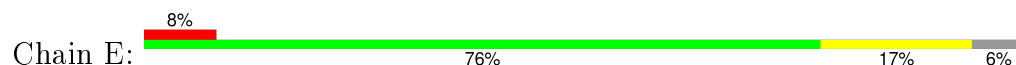




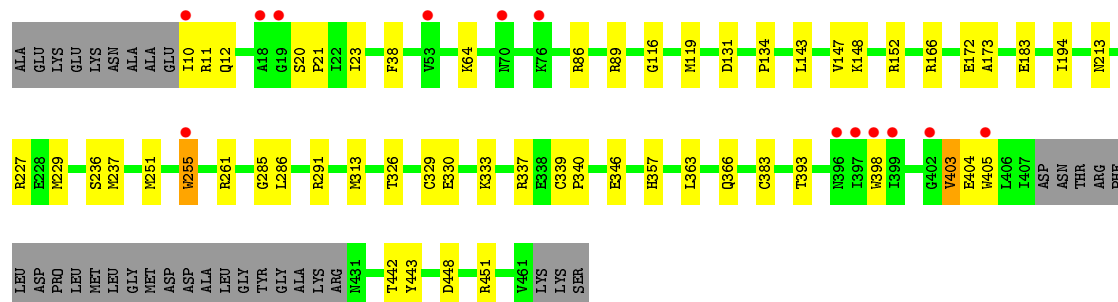
• Molecule 1: TETRACHLOROETHENE REDUCTIVE DEHALOGENASE CATALYTIC SUB-UNIT



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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 0.186 , 0.221	Depositor DCC
R_{free} test set	6850 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	27.7	Xtriage
Anisotropy	0.219	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 51.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	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.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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, 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 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	3608	0	3505	37	0
1	B	3443	0	3329	31	0
1	C	3497	0	3386	37	0
1	D	3444	0	3334	35	0
1	E	3436	0	3322	63	0
1	F	3385	0	3282	44	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	82	4	0
3	B	89	0	82	4	0
3	C	89	0	82	9	0
3	D	89	0	82	6	0
3	E	89	0	82	9	0
3	F	89	0	82	8	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	20650	247	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 6.

All (247) 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)
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: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:364:GLN:HE21	1:A:366:GLN:HE22	1.33	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:F:64:LYS:NZ	4:F:2027:HOH:O	2.27	0.68
1:B:313:MET:SD	4:B:2147:HOH:O	2.50	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:451:ARG:HD2	1:F:451:ARG:HH21	1.61	0.65
1:E:456:PHE:HB3	1:E:458:LYS:HE2	1.77	0.65
1:F:172:GLU:OE2	4:F:2079:HOH:O	2.14	0.64
3:D:503:BVQ:H35	3:D:503:BVQ:H36A	1.80	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
3:F:503:BVQ:H36A	3:F:503:BVQ:H35	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
3:E:503:BVQ:H35	3:E:503:BVQ:H36A	1.83	0.61
3:A:503:BVQ:H36A	3:A:503:BVQ:H35	1.81	0.60
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:E:38:PHE:CD2	3:E:503:BVQ:H53A	2.37	0.60
3:B:503:BVQ:H36A	3:B:503:BVQ:H35	1.82	0.60
3:C:503:BVQ:H35	3:C:503:BVQ:H36A	1.84	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: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:B:227:ARG:NH1	1:B:393:THR:O	2.35	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
3:C:503:BVQ:H55A	3:C:503:BVQ:H53	1.86	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:431:ASN:N	4:C:2234:HOH:O	2.37	0.57
3:A:503:BVQ:H53	3:A:503:BVQ:H55A	1.87	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
3:D:503:BVQ:H55A	3:D:503:BVQ:H53	1.89	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
1:E:401:ASP:OD2	1:E:404:GLU:HG2	2.08	0.53
1:C:86:ARG:HD2	1:D:136:ASP:OD2	2.09	0.53
1:A:264:GLY:HA2	4:A:2077:HOH:O	2.09	0.53
1:E:251[A]:MET:SD	1:F:251:MET:HG3	2.49	0.53
1:A:98:LEU:CD2	1:A:251:MET:HG2	2.39	0.53
1:F:366:GLN:NE2	4:F:2120:HOH:O	2.31	0.53
1:C:364:GLN:HE21	1:C:366:GLN:HE22	1.57	0.53
3:B:503:BVQ:H55A	3:B:503:BVQ:H53	1.91	0.53
1:C:313:MET:HE2	1:C:315:LEU:HD21	1.91	0.53
1:C:76:LYS:O	1:C:76:LYS:HG3	2.07	0.53
1:B:333:LYS:HB2	1:B:337:ARG:HH11	1.73	0.53
3:E:503:BVQ:H55A	3:E:503:BVQ:H53	1.89	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:B:333:LYS:HB2	1:B:337:ARG:NH1	2.26	0.51
1:A:213:ASN:ND2	4:A:2105:HOH:O	2.33	0.51
1:F:38:PHE:CD2	3:F:503:BVQ:H53A	2.45	0.51
1:E:457:ARG:HB3	4:E:2096:HOH:O	2.10	0.51
1:E:357:HIS:O	3:E:503:BVQ:H2PA	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:F:147:VAL:HB	1:F:313:MET:HE2	1.92	0.50
1:A:397:ILE:HD11	1:A:412:PHE:CZ	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:173:ALA:HB2	1:D:194:ILE:HD11	1.93	0.50
1:D:38:PHE:CD2	3:D:503:BVQ:H53A	2.46	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:D:231:GLN:NE2	4:D:2131:HOH:O	2.45	0.49
1:B:270:SER:OG	1:B:308:LYS:HG3	2.11	0.49
1:D:6:ASN:HB3	1:D:9:GLU:OE1	2.13	0.49
1:E:227:ARG:O	1:E:231:GLN:HG2	2.12	0.49
1:A:401:ASP:OD1	1:A:402:GLY:N	2.45	0.49
1:E:266:TYR:CZ	1:E:312:ASN:HB3	2.48	0.49
1:C:368:ASP:OD2	4:C:2222:HOH:O	2.20	0.49
1:B:13:GLN:OE1	1:B:405:TRP:HB2	2.12	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:F:38:PHE:CZ	3:F:503:BVQ:H46A	2.48	0.48
1:E:199:VAL:HG21	1:E:203:ILE:HD13	1.94	0.48
1:E:451:ARG:NH2	1:F:448:ASP:HA	2.29	0.48
1:A:323:PHE:HD2	1:A:407:ILE:HD11	1.78	0.48
1:E:246:TYR:O	1:E:249:MET:HB2	2.14	0.48
1:F:166:ARG:NH2	1:F:213:ASN:OD1	2.44	0.47
1:A:154:ALA:HA	1:A:255:TRP:CE3	2.49	0.47
1:C:261:ARG:HA	1:C:265:TYR:O	2.14	0.47
1:E:353:GLY:HA2	1:E:366:GLN:HG2	1.97	0.47
1:C:337:ARG:NH2	1:C:414:ASP:OD2	2.48	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:38:PHE:CD2	3:A:503:BVQ:H53A	2.50	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:E:364:GLN:HE22	3:E:503:BVQ:P	2.38	0.46
1:A:5:LYS:HA	1:A:405:TRP:CH2	2.50	0.46
1:F:333:LYS:HB2	1:F:337:ARG:NH1	2.30	0.46
3:F:503:BVQ:H25B	3:F:503:BVQ:H30	1.78	0.46
1:E:442:THR:HG22	1:E:443:TYR:CD2	2.50	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:A:23:ILE:HD11	1:A:363:LEU:HD23	1.97	0.46
1:E:451:ARG:NH1	1:F:451:ARG:HH22	2.13	0.46
1:E:270:SER:OG	1:E:308:LYS:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:ARG:HA	1:B:265:TYR:O	2.15	0.46
1:F:229:MET:HB3	1:F:237:MET:O	2.16	0.46
1:C:38:PHE:CD2	3:C:503:BVQ:H53A	2.50	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:F:357:HIS:O	3:F:503:BVQ:H2P	2.16	0.45
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
3:F:503:BVQ:H60	3:F:503:BVQ:H25A	1.98	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:E:38:PHE:HD2	3:E:503:BVQ:H53A	1.80	0.45
1:B:45:PHE:HD2	1:B:53:VAL:HG12	1.81	0.45
1:A:261:ARG:HA	1:A:265:TYR:O	2.16	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: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:449:HIS:ND1	4:A:2188:HOH:O	2.36	0.45
1:A:251:MET:HE2	1:B:251[B]:MET:SD	2.56	0.44
1:A:195:VAL:HG21	1:A:197:LYS:HE3	1.99	0.44
1:A:136:ASP:OD2	1:B:86:ARG:HD2	2.18	0.44
3:F:503:BVQ:H47	3:F:503:BVQ:H48A	1.92	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
1:F:326:THR:O	1:F:330:GLU:HG3	2.17	0.44
1:E:344:ILE:O	4:E:2083:HOH:O	2.21	0.44
1:D:139:ASP:HA	1:D:140:PRO:HD2	1.83	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
3:D:503:BVQ:H26A	3:D:503:BVQ:H19	1.81	0.44
3:E:503:BVQ:H30	3:E:503:BVQ:H25B	1.68	0.44
1:B:352:GLU:OE2	4:B:2018:HOH:O	2.21	0.44
1:B:55:PRO:HD2	1:B:58:LEU:HD12	2.00	0.44
1:B:398:TRP:CZ3	1:B:407:ILE:HG13	2.53	0.44
1:C:323:PHE:HD2	1:C:407:ILE:HD11	1.82	0.44
1:C:38:PHE:CZ	3:C:503:BVQ:H46A	2.53	0.43
1:E:147:VAL:HG21	1:E:313:MET:HE3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:280:PHE:CD2	1:C:308:LYS:HD2	2.53	0.43
1:E:133:ARG:HA	1:E:134:PRO:HD3	1.90	0.43
1:C:440:ILE:HG13	1:C:441:ASN:N	2.33	0.43
1:F:398:TRP:HB3	1:F:405:TRP:CE3	2.53	0.43
1:F:339:CYS:HA	1:F:340:PRO:HD3	1.78	0.43
1:C:116:GLY:HA2	1:C:119:MET:CE	2.48	0.43
1:B:342:LYS:HD3	1:B:342:LYS:HA	1.72	0.43
1:D:372:CYS:SG	3:D:503:BVQ:H47A	2.58	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:372:CYS:SG	3:B:503:BVQ:H47A	2.59	0.43
1:E:181:PRO:HD2	1:E:184:GLN:OE1	2.19	0.43
1:D:313:MET:HA	1:D:314:PRO:HD3	1.91	0.43
1:C:223:ILE:HG23	1:C:248:ARG:CZ	2.49	0.43
1:B:103:GLY:O	1:B:272:ASN:HB2	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:C:123:GLN:OE1	1:D:183:GLU:HG3	2.19	0.43
1:F:173:ALA:HB2	1:F:194:ILE:HD11	2.01	0.43
1:C:372:CYS:SG	3:C:503:BVQ:H47A	2.59	0.42
3:C:503:BVQ:H48A	3:C:503:BVQ:H47	1.94	0.42
1:B:451:ARG:O	1:B:454:VAL:HG12	2.18	0.42
3:C:503:BVQ:H30	3:C:503:BVQ:H25B	1.86	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:E:75:PRO:O	1:E:76:LYS:CB	2.67	0.42
1:D:48:ASN:OD1	1:D:52:GLU:HG3	2.19	0.42
3:E:503:BVQ:H60	3:E:503:BVQ:H26A	2.02	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
3:D:503:BVQ:H60	3:D:503:BVQ:H25A	2.02	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
1:D:98:LEU:CD2	1:D:251:MET:HG2	2.50	0.41
1:C:293:GLY:O	3:C:503:BVQ:H1R	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:148:LYS:O	1:E:152:ARG:HG2	2.21	0.41
1:D:196:PHE:HA	1:D:211:ILE:O	2.21	0.41
1:F:148:LYS:O	1:F: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:A:148:LYS:O	1:A:152:ARG:HG2	2.20	0.41
1:E:133:ARG:HG2	1:F:86:ARG:HH12	1.85	0.41
1:C:394:LYS:NZ	1:C:411:ARG:O	2.51	0.41
1:C:76:LYS:O	1:C:76:LYS:CG	2.69	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
3:C:503:BVQ:H18	3:C:503:BVQ:H56A	1.93	0.41
1:A:143:LEU:HD13	1:A:313:MET:HG3	2.02	0.41
3:F:503:BVQ:H26A	3:F:503:BVQ:H19	1.85	0.40
3:A:503:BVQ:H18	3:A:503:BVQ:H56A	1.94	0.40
3:B:503:BVQ:H60	3:B:503:BVQ:H25A	2.03	0.40
1:B:296:ILE:HG23	1:B:301:GLY:HA2	2.03	0.40
1:A:177:PRO:HG2	1:A:180:VAL:CG2	2.51	0.40
3:E:503:BVQ:H56A	3:E:503:BVQ:H18	1.80	0.40
1:E:199:VAL:HG21	1:E:203:ILE:CD1	2.51	0.40
1:E:440:ILE:HA	1:E:440:ILE:HD12	1.88	0.40
1:D:461:VAL:C	1:D:462:LYS:HD2	2.41	0.40
1:F:20:SER:HA	1:F:21:PRO:HD2	1.93	0.40
1:C:40:HIS:CE1	1:C:42:THR:HG1	2.38	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%)	52	60
1	B	433/464 (93%)	415 (96%)	16 (4%)	2 (0%)	34	34
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%)	52	60
1	F	425/464 (92%)	412 (97%)	12 (3%)	1 (0%)	52	60
All	All	2618/2784 (94%)	2528 (97%)	85 (3%)	5 (0%)	52	60

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%)	92	95
1	C	374/389 (96%)	373 (100%)	1 (0%)	94	97
1	D	368/389 (95%)	367 (100%)	1 (0%)	94	97
1	E	367/389 (94%)	365 (100%)	2 (0%)	92	95
1	F	362/389 (93%)	360 (99%)	2 (1%)	90	94
All	All	2223/2334 (95%)	2215 (100%)	8 (0%)	94	96

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
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 [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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	A	502	1	0,12,12	0.00	-	0,24,24	0.00	-
3	BVQ	A	503	4	70,99,99	0.55	0	99,162,162	1.27	12 (12%)
2	SF4	B	501	1	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	B	502	1	0,12,12	0.00	-	0,24,24	0.00	-
3	BVQ	B	503	4	70,99,99	0.57	1 (1%)	99,162,162	1.41	12 (12%)
2	SF4	C	501	1	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	C	502	1	0,12,12	0.00	-	0,24,24	0.00	-
3	BVQ	C	503	-	70,99,99	0.57	1 (1%)	99,162,162	1.34	10 (10%)
2	SF4	D	501	1	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	D	502	1	0,12,12	0.00	-	0,24,24	0.00	-
3	BVQ	D	503	4	70,99,99	0.54	0	99,162,162	1.33	13 (13%)
2	SF4	E	501	1	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	E	502	1	0,12,12	0.00	-	0,24,24	0.00	-
3	BVQ	E	503	4	70,99,99	0.57	1 (1%)	99,162,162	1.35	14 (14%)
2	SF4	F	501	1	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	F	502	1	0,12,12	0.00	-	0,24,24	0.00	-
3	BVQ	F	503	-	70,99,99	0.55	1 (1%)	99,162,162	1.26	11 (11%)

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	3/3/35/37	0/49/221/221	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	3/3/35/37	0/49/221/221	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	-	3/3/35/37	0/49/221/221	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	3/3/35/37	0/49/221/221	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	3/3/35/37	0/49/221/221	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	-	3/3/35/37	0/49/221/221	0/3/11/11

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	503	BVQ	P-O5	2.05	1.53	1.48
3	E	503	BVQ	P-O5	2.10	1.53	1.48
3	C	503	BVQ	P-O5	2.13	1.53	1.48
3	F	503	BVQ	P-O5	2.18	1.53	1.48

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	503	BVQ	C30-C3-C2	-3.97	111.25	119.11
3	A	503	BVQ	C35-C5-C4	-3.75	111.53	118.25
3	C	503	BVQ	C35-C5-C4	-3.65	111.71	118.25
3	F	503	BVQ	C35-C5-C4	-3.63	111.74	118.25
3	D	503	BVQ	C35-C5-C4	-3.58	111.83	118.25
3	E	503	BVQ	C35-C5-C4	-3.46	112.06	118.25
3	B	503	BVQ	C35-C5-C4	-3.45	112.07	118.25
3	F	503	BVQ	C30-C3-C2	-3.36	112.46	119.11
3	E	503	BVQ	C9-C10-C11	-3.31	123.99	132.28
3	F	503	BVQ	C9-C10-C11	-3.30	124.00	132.28
3	C	503	BVQ	C9-C10-C11	-3.28	124.05	132.28
3	E	503	BVQ	C55-C17-C18	-3.25	104.46	110.97
3	A	503	BVQ	C9-C10-C11	-3.24	124.16	132.28
3	B	503	BVQ	C9-C10-C11	-3.20	124.26	132.28
3	C	503	BVQ	C30-C3-C2	-3.16	112.87	119.11
3	D	503	BVQ	C9-C10-C11	-3.11	124.48	132.28
3	A	503	BVQ	C30-C3-C2	-2.97	113.23	119.11
3	E	503	BVQ	C56-C55-C17	-2.85	109.61	115.57
3	B	503	BVQ	C30-C3-C2	-2.81	113.55	119.11
3	B	503	BVQ	C20-C1-C19	-2.77	106.67	109.38
3	D	503	BVQ	C30-C3-C2	-2.74	113.69	119.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	503	BVQ	C13-C14-C15	-2.64	122.97	131.88
3	F	503	BVQ	C55-C17-C18	-2.60	105.76	110.97
3	F	503	BVQ	C13-C14-C15	-2.58	123.17	131.88
3	D	503	BVQ	C36-C7-C8	-2.57	107.58	112.24
3	D	503	BVQ	C55-C17-C18	-2.55	105.86	110.97
3	D	503	BVQ	C13-C14-C15	-2.54	123.32	131.88
3	E	503	BVQ	C3-C4-C5	-2.53	123.33	131.88
3	C	503	BVQ	C3-C4-C5	-2.53	123.34	131.88
3	D	503	BVQ	C3-C4-C5	-2.52	123.36	131.88
3	F	503	BVQ	C3-C4-C5	-2.52	123.36	131.88
3	B	503	BVQ	C13-C14-C15	-2.52	123.37	131.88
3	A	503	BVQ	C3-C4-C5	-2.45	123.61	131.88
3	B	503	BVQ	C3-C4-C5	-2.42	123.70	131.88
3	A	503	BVQ	C13-C14-C15	-2.42	123.72	131.88
3	E	503	BVQ	C13-C14-C15	-2.39	123.81	131.88
3	E	503	BVQ	C48-C13-C12	-2.28	110.28	116.53
3	A	503	BVQ	C20-C1-C19	-2.24	107.18	109.38
3	A	503	BVQ	C55-C17-C18	-2.19	106.57	110.97
3	F	503	BVQ	C20-C1-C19	-2.17	107.25	109.38
3	A	503	BVQ	C36-C7-C8	-2.13	108.38	112.24
3	D	503	BVQ	C1-C19-C18	-2.09	118.18	121.85
3	D	503	BVQ	C20-C1-C19	-2.08	107.34	109.38
3	B	503	BVQ	C55-C17-C18	-2.06	106.83	110.97
3	C	503	BVQ	C55-C17-C18	-2.01	106.94	110.97
3	E	503	BVQ	C41-C8-C7	2.00	119.87	114.16
3	D	503	BVQ	C10-C9-N22	2.00	129.38	124.15
3	E	503	BVQ	C53-C15-C14	2.01	121.84	118.25
3	B	503	BVQ	C10-C9-N22	2.05	129.50	124.15
3	B	503	BVQ	C19-C1-N21	2.05	104.25	102.16
3	C	503	BVQ	C10-C9-N22	2.08	129.57	124.15
3	F	503	BVQ	C10-C9-N22	2.08	129.59	124.15
3	E	503	BVQ	P-O3-C2P	2.17	126.94	118.48
3	A	503	BVQ	P-O3-C2P	2.20	127.08	118.48
3	B	503	BVQ	P-O2-C3R	2.41	127.22	120.07
3	F	503	BVQ	P-O2-C3R	2.42	127.26	120.07
3	F	503	BVQ	C1R-N1B-C8B	2.45	129.82	125.57
3	E	503	BVQ	P-O2-C3R	2.55	127.63	120.07
3	D	503	BVQ	P-O2-C3R	2.60	127.78	120.07
3	A	503	BVQ	P-O2-C3R	2.64	127.91	120.07
3	C	503	BVQ	P-O2-C3R	2.85	128.53	120.07
3	A	503	BVQ	C1R-N1B-C8B	3.55	131.72	125.57
3	E	503	BVQ	C1R-N1B-C8B	3.86	132.27	125.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	503	BVQ	C35-C5-C6	4.50	126.31	118.25
3	C	503	BVQ	C35-C5-C6	4.58	126.45	118.25
3	F	503	BVQ	C35-C5-C6	4.64	126.56	118.25
3	B	503	BVQ	C35-C5-C6	4.70	126.66	118.25
3	D	503	BVQ	C35-C5-C6	4.77	126.79	118.25
3	A	503	BVQ	C35-C5-C6	4.98	127.16	118.25
3	D	503	BVQ	C1R-N1B-C8B	5.50	135.11	125.57
3	C	503	BVQ	C1R-N1B-C8B	6.64	137.10	125.57
3	B	503	BVQ	C1R-N1B-C8B	7.16	138.00	125.57

All (18) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	C	503	BVQ	N24
3	C	503	BVQ	N23
3	C	503	BVQ	N21
3	E	503	BVQ	N24
3	E	503	BVQ	N23
3	E	503	BVQ	N21
3	D	503	BVQ	N24
3	D	503	BVQ	N23
3	D	503	BVQ	N21
3	A	503	BVQ	N24
3	A	503	BVQ	N23
3	A	503	BVQ	N21
3	F	503	BVQ	N24
3	F	503	BVQ	N23
3	F	503	BVQ	N21
3	B	503	BVQ	N24
3	B	503	BVQ	N23
3	B	503	BVQ	N21

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	503	BVQ	4	0
3	B	503	BVQ	4	0
3	C	503	BVQ	9	0
3	D	503	BVQ	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	502	SF4	1	0
3	E	503	BVQ	9	0
2	F	502	SF4	1	0
3	F	503	BVQ	8	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	458/464 (98%)	0.07	19 (4%) 41 43	20, 35, 53, 67	0
1	B	436/464 (93%)	0.14	37 (8%) 13 14	18, 29, 53, 87	0
1	C	442/464 (95%)	-0.19	4 (0%) 85 86	14, 25, 43, 73	0
1	D	437/464 (94%)	-0.02	20 (4%) 36 38	14, 26, 56, 94	0
1	E	435/464 (93%)	0.41	36 (8%) 14 15	22, 46, 67, 85	0
1	F	429/464 (92%)	-0.07	13 (3%) 54 57	21, 38, 61, 77	0
All	All	2637/2784 (94%)	0.06	129 (4%) 33 35	14, 33, 59, 94	0

All (129) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	410	THR	8.6
1	D	403	VAL	7.5
1	E	396	ASN	7.3
1	E	403	VAL	6.7
1	B	403	VAL	6.6
1	F	396	ASN	6.6
1	D	407	ILE	6.5
1	D	399	ILE	6.4
1	D	405	TRP	6.4
1	F	397	ILE	5.8
1	E	408	ASP	5.8
1	D	396	ASN	5.7
1	D	398	TRP	5.6
1	B	251[A]	MET	5.4
1	D	401	ASP	5.3
1	E	395	GLY	5.2
1	E	402	GLY	5.1
1	B	407	ILE	5.0
1	E	26	ASP	5.0

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Mol	Chain	Res	Type	RSRZ
1	B	402	GLY	5.0
1	B	404	GLU	4.9
1	E	399	ILE	4.6
1	D	409	ASN	4.6
1	D	400	HIS	4.4
1	D	397	ILE	4.2
1	D	6	ASN	4.2
1	D	404	GLU	4.2
1	B	401	ASP	4.1
1	B	400	HIS	4.0
1	E	401	ASP	4.0
1	D	395	GLY	3.9
1	D	406	LEU	3.8
1	D	402	GLY	3.7
1	F	405	TRP	3.7
1	E	76	LYS	3.7
1	F	398	TRP	3.5
1	E	24	VAL	3.5
1	E	397	ILE	3.5
1	E	53	VAL	3.5
1	B	399	ILE	3.5
1	F	18	ALA	3.4
1	A	18	ALA	3.3
1	A	403	VAL	3.3
1	F	76	LYS	3.2
1	F	10	ILE	3.2
1	D	394	LYS	3.2
1	F	19	GLY	3.1
1	B	410	THR	3.1
1	C	76	LYS	3.1
1	E	406	LEU	3.1
1	D	408	ASP	3.1
1	E	28	LEU	3.0
1	B	443	TYR	3.0
1	B	6	ASN	3.0
1	F	399	ILE	3.0
1	A	154	ALA	3.0
1	F	255	TRP	2.9
1	A	70	ASN	2.9
1	C	251[A]	MET	2.9
1	E	409	ASN	2.8
1	F	402	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	395	GLY	2.8
1	B	250	CYS	2.8
1	E	59	SER	2.7
1	B	249	MET	2.7
1	D	9	GLU	2.7
1	E	51	GLY	2.7
1	E	365	TRP	2.7
1	E	23	ILE	2.6
1	B	19	GLY	2.6
1	E	394	LYS	2.6
1	B	255	TRP	2.6
1	B	97	THR	2.5
1	E	16	MET	2.5
1	B	98	LEU	2.5
1	B	223	ILE	2.5
1	B	244	PHE	2.5
1	A	26	ASP	2.5
1	A	69	GLU	2.5
1	B	18	ALA	2.5
1	B	405	TRP	2.4
1	B	408	ASP	2.4
1	B	76	LYS	2.4
1	E	371	LYS	2.4
1	B	252	PHE	2.4
1	E	352	GLU	2.3
1	E	404	GLU	2.3
1	B	26	ASP	2.3
1	A	255	TRP	2.3
1	E	354	ARG	2.3
1	B	397	ILE	2.3
1	E	328	PHE	2.3
1	A	19	GLY	2.3
1	B	247	SER	2.3
1	E	398	TRP	2.3
1	B	396	ASN	2.3
1	A	98	LEU	2.3
1	C	415	PRO	2.3
1	E	363	LEU	2.3
1	A	443	TYR	2.2
1	B	245	CYS	2.2
1	A	252	PHE	2.2
1	E	400	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	53	VAL	2.2
1	E	45	PHE	2.2
1	E	405	TRP	2.2
1	A	17	THR	2.2
1	B	307	THR	2.2
1	F	70	ASN	2.2
1	B	154	ALA	2.2
1	A	462	LYS	2.1
1	B	132	ARG	2.1
1	D	10	ILE	2.1
1	A	50	LYS	2.1
1	A	45	PHE	2.1
1	C	256	LEU	2.1
1	E	247	SER	2.1
1	B	406	LEU	2.1
1	B	50	LYS	2.1
1	B	155	GLY	2.1
1	E	151	ALA	2.1
1	A	76	LYS	2.1
1	E	52	GLU	2.1
1	A	248	ARG	2.0
1	E	251[A]	MET	2.0
1	A	51	GLY	2.0
1	E	337	ARG	2.0
1	B	224	ALA	2.0
1	B	9	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 carbohydrates 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. 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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	BVQ	C	503	89/89	0.97	0.12	0.18	13,21,28,32	0
3	BVQ	B	503	89/89	0.97	0.13	0.02	12,22,27,30	0
3	BVQ	D	503	89/89	0.96	0.12	-0.08	14,21,26,36	0
3	BVQ	F	503	89/89	0.97	0.11	-0.12	19,29,36,50	0
3	BVQ	A	503	89/89	0.96	0.11	-0.42	21,30,36,38	0
2	SF4	C	502	8/8	0.98	0.09	-0.47	19,23,24,25	0
3	BVQ	E	503	89/89	0.94	0.12	-0.47	29,42,49,59	0
2	SF4	D	502	8/8	0.99	0.09	-0.59	22,24,26,29	0
2	SF4	C	501	8/8	0.99	0.08	-1.19	19,23,25,28	0
2	SF4	F	501	8/8	0.97	0.06	-1.60	33,38,41,44	0
2	SF4	E	501	8/8	0.96	0.06	-1.61	43,51,52,53	0
2	SF4	B	501	8/8	0.99	0.06	-1.76	20,24,25,28	0
2	SF4	A	502	8/8	0.98	0.06	-1.79	29,32,35,36	0
2	SF4	D	501	8/8	0.99	0.05	-1.83	19,26,28,30	0
2	SF4	B	502	8/8	0.99	0.05	-1.83	20,23,24,24	0
2	SF4	F	502	8/8	0.97	0.08	-1.89	32,35,39,39	0
2	SF4	A	501	8/8	0.97	0.06	-1.95	28,32,34,38	0
2	SF4	E	502	8/8	0.96	0.06	-2.24	38,47,52,54	0

6.5 Other polymers [i](#)

There are no such residues in this entry.