



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 15, 2017 – 10:01 AM EDT

PDB ID : 5TUW
Title : Crystal structure of Orange Carotenoid Protein with partial loss of 3'OH Echinone chromophore
Authors : Yang, X.; Bandara, S.; Ren, Z.
Deposited on : unknown
Resolution : 2.30 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029824
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20029824

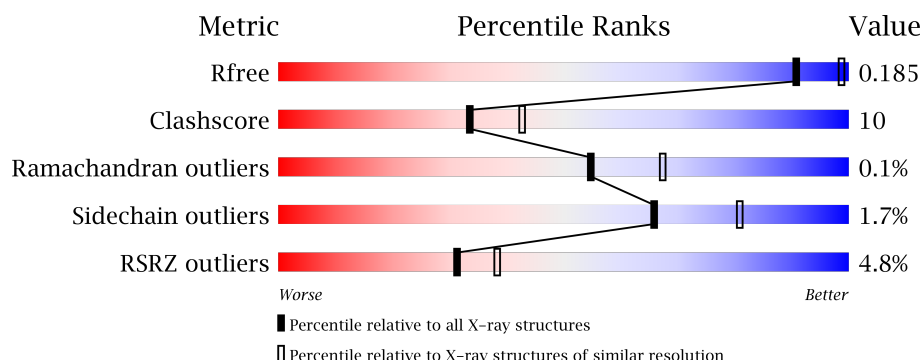
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	100719	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

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	323	<div> <div>4%</div> <div>76% 17% • 6%</div> </div>
1	B	323	<div> <div>5%</div> <div>79% 14% • 6%</div> </div>
1	C	323	<div> <div>6%</div> <div>72% 22% • 6%</div> </div>
1	D	323	<div> <div>3%</div> <div>81% 13% 5%</div> </div>
1	E	323	<div> <div>5%</div> <div>73% 20% • 6%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	323	

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	EQ3	A	402	-	-	-	X
3	EQ3	B	401	-	-	-	X
3	EQ3	C	403	-	-	-	X
3	EQ3	D	401	-	-	-	X
3	EQ3	E	402	-	-	-	X
3	EQ3	F	401	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15054 atoms, of which 356 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 Orange carotenoid-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	305	Total	C	N	O	S	0	2	0
			2357	1508	397	441	11			
1	B	304	Total	C	N	O	S	0	3	0
			2359	1510	396	442	11			
1	C	305	Total	C	N	O	S	0	2	0
			2359	1508	397	443	11			
1	D	306	Total	C	N	O	S	0	3	0
			2368	1515	398	444	11			
1	E	305	Total	C	N	O	S	0	2	0
			2359	1508	397	443	11			
1	F	305	Total	C	N	O	S	0	2	0
			2357	1508	396	442	11			

There are 36 discrepancies between the modelled and reference sequences:

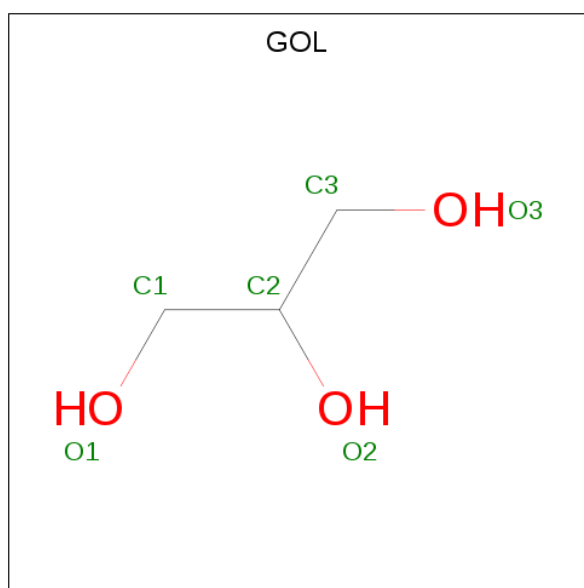
Chain	Residue	Modelled	Actual	Comment	Reference
A	318	HIS	-	expression tag	UNP P74102
A	319	HIS	-	expression tag	UNP P74102
A	320	HIS	-	expression tag	UNP P74102
A	321	HIS	-	expression tag	UNP P74102
A	322	HIS	-	expression tag	UNP P74102
A	323	HIS	-	expression tag	UNP P74102
B	318	HIS	-	expression tag	UNP P74102
B	319	HIS	-	expression tag	UNP P74102
B	320	HIS	-	expression tag	UNP P74102
B	321	HIS	-	expression tag	UNP P74102
B	322	HIS	-	expression tag	UNP P74102
B	323	HIS	-	expression tag	UNP P74102
C	318	HIS	-	expression tag	UNP P74102
C	319	HIS	-	expression tag	UNP P74102
C	320	HIS	-	expression tag	UNP P74102
C	321	HIS	-	expression tag	UNP P74102
C	322	HIS	-	expression tag	UNP P74102

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Chain	Residue	Modelled	Actual	Comment	Reference
C	323	HIS	-	expression tag	UNP P74102
D	318	HIS	-	expression tag	UNP P74102
D	319	HIS	-	expression tag	UNP P74102
D	320	HIS	-	expression tag	UNP P74102
D	321	HIS	-	expression tag	UNP P74102
D	322	HIS	-	expression tag	UNP P74102
D	323	HIS	-	expression tag	UNP P74102
E	318	HIS	-	expression tag	UNP P74102
E	319	HIS	-	expression tag	UNP P74102
E	320	HIS	-	expression tag	UNP P74102
E	321	HIS	-	expression tag	UNP P74102
E	322	HIS	-	expression tag	UNP P74102
E	323	HIS	-	expression tag	UNP P74102
F	318	HIS	-	expression tag	UNP P74102
F	319	HIS	-	expression tag	UNP P74102
F	320	HIS	-	expression tag	UNP P74102
F	321	HIS	-	expression tag	UNP P74102
F	322	HIS	-	expression tag	UNP P74102
F	323	HIS	-	expression tag	UNP P74102

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



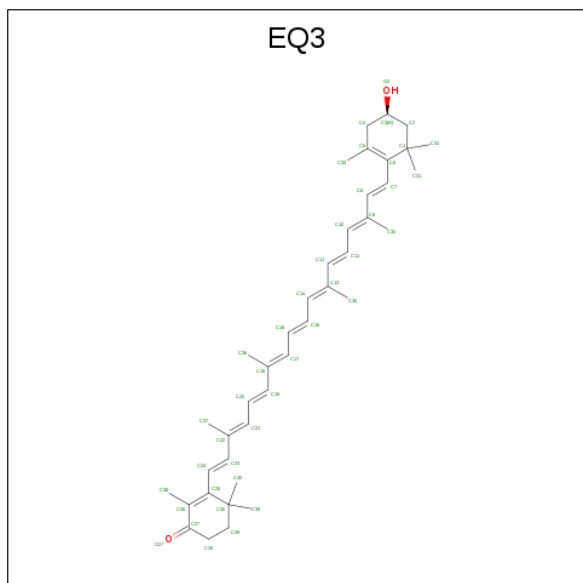
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	C	1	Total	C	H	O	0	0
			14	3	8	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	H	O	0	0
			14	3	8	3		
2	E	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 3 is (3'R)-3'-hydroxy-beta,beta-caroten-4-one (three-letter code: EQ3) (formula: $C_{40}H_{54}O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			96	40	54	2		
3	B	1	Total	C	H	O	0	0
			96	40	54	2		
3	C	1	Total	C	H	O	0	0
			96	40	54	2		
3	D	1	Total	C	H	O	0	0
			96	40	54	2		
3	E	1	Total	C	H	O	0	0
			96	40	54	2		
3	F	1	Total	C	H	O	0	0
			96	40	54	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	48	Total	O	0	0
			48	48		

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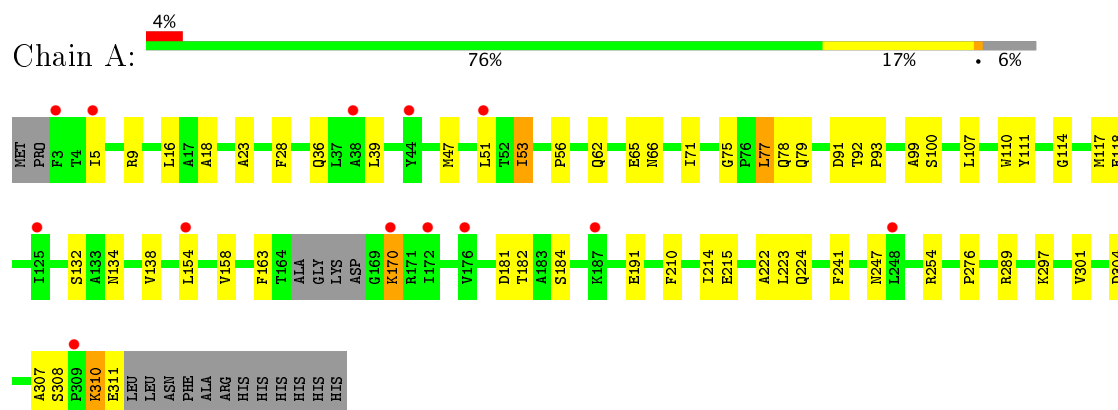
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	39	Total 39	O 39	0	0
4	C	42	Total 42	O 42	0	0
4	D	38	Total 38	O 38	0	0
4	E	49	Total 49	O 49	0	0
4	F	47	Total 47	O 47	0	0

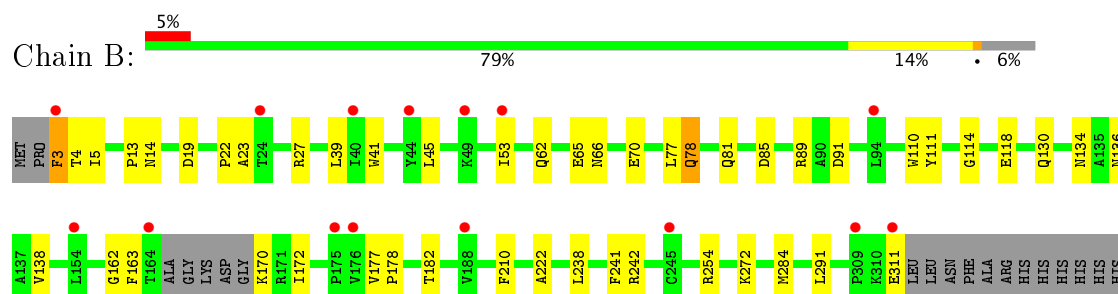
3 Residue-property plots [i](#)

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

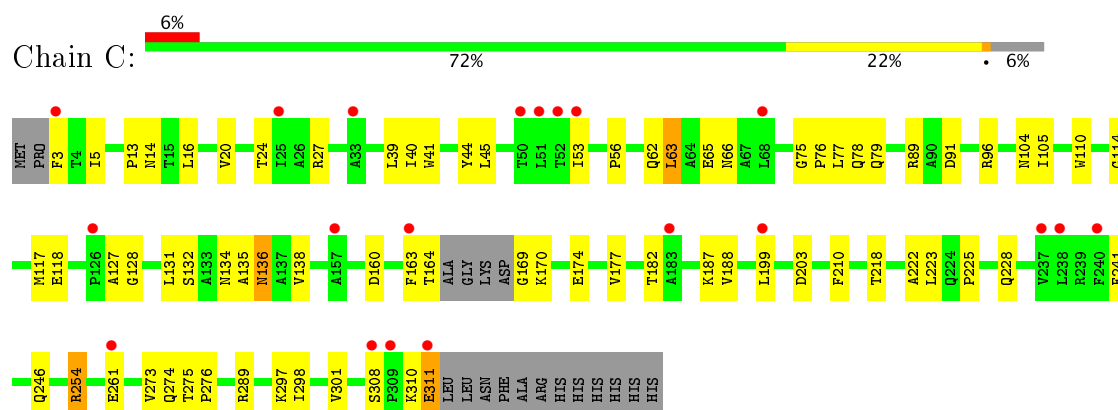
- Molecule 1: Orange carotenoid-binding protein



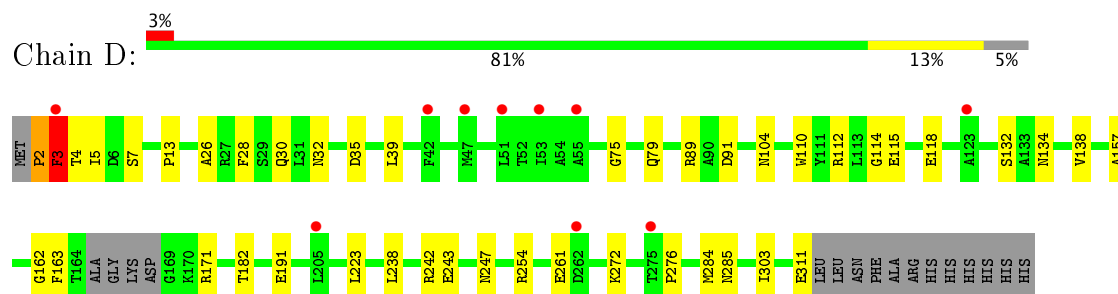
- Molecule 1: Orange carotenoid-binding protein



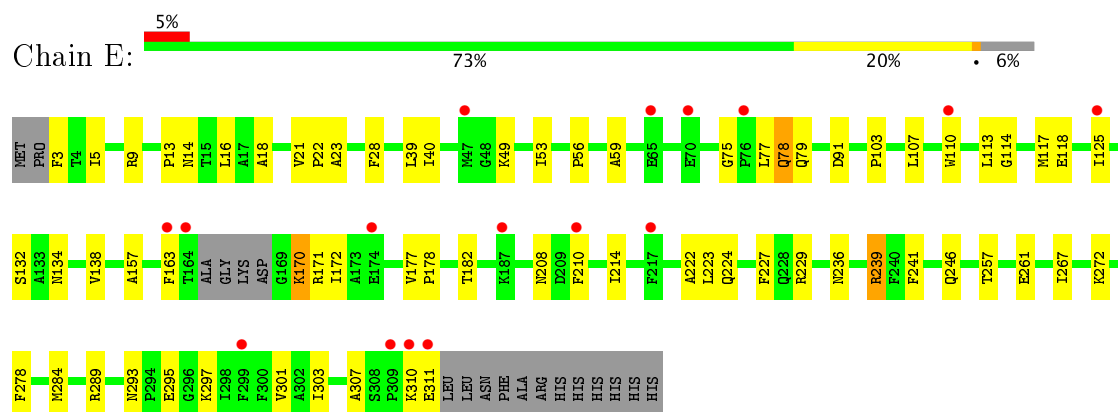
- Molecule 1: Orange carotenoid-binding protein



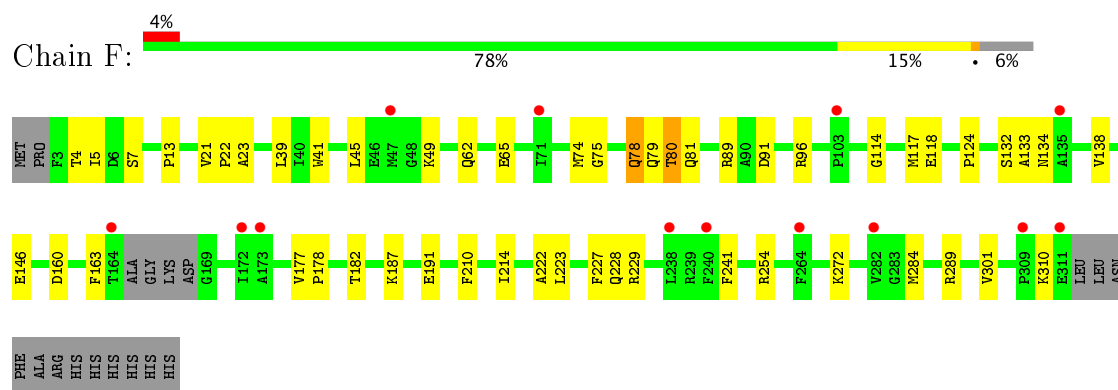
- Molecule 1: Orange carotenoid-binding protein



- Molecule 1: Orange carotenoid-binding protein



- Molecule 1: Orange carotenoid-binding protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	82.95Å 82.91Å 87.44Å 89.79° 89.91° 60.04°	Depositor
Resolution (Å)	41.49 – 2.30 41.49 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.3 (41.49-2.30) 95.0 (41.49-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 2.29Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.185 , 0.239 0.185 , 0.185	Depositor DCC
R_{free} test set	4090 reflections (4.79%)	DCC
Wilson B-factor (Å ²)	41.3	Xtriage
Anisotropy	0.210	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 100.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.016 for h-k,h,l 0.016 for k,-h+k,l 0.396 for -k,h-k,l 0.396 for -h+k,-h,l 0.428 for -h+k,k,-l 0.399 for h,h-k,-l 0.021 for -h,-k,l 0.021 for k,h,-l 0.418 for -k,-h,-l 0.019 for h-k,-k,-l 0.017 for -h,-h+k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15054	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.82% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, EQ3

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	0.44	0/2412	0.60	0/3283
1	B	0.44	0/2417	0.60	0/3290
1	C	0.48	1/2414 (0.0%)	0.61	1/3285 (0.0%)
1	D	0.44	0/2426	0.61	1/3302 (0.0%)
1	E	0.44	0/2414	0.61	0/3285
1	F	0.44	0/2412	0.59	0/3283
All	All	0.45	1/14495 (0.0%)	0.61	2/19728 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	311	GLU	CB-CG	-6.61	1.39	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	2	PRO	N-CA-CB	6.33	110.90	103.30
1	C	27	ARG	NE-CZ-NH1	-5.71	117.45	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2357	0	2360	49	0
1	B	2359	0	2363	40	0
1	C	2359	0	2357	63	0
1	D	2368	0	2368	32	0
1	E	2359	0	2357	60	0
1	F	2357	0	2358	46	0
2	A	6	8	8	1	0
2	C	12	16	16	4	0
2	E	6	8	8	1	0
3	A	42	54	0	1	0
3	B	42	54	0	1	0
3	C	42	54	0	2	0
3	D	42	54	0	1	0
3	E	42	54	0	2	0
3	F	42	54	0	0	0
4	A	48	0	0	2	0
4	B	39	0	0	1	0
4	C	42	0	0	7	0
4	D	38	0	0	2	0
4	E	49	0	0	3	0
4	F	47	0	0	12	0
All	All	14698	356	14195	277	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 10.

All (277) 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:B:14:ASN:ND2	1:E:14:ASN:OD1	1.96	0.99
1:F:89:ARG:NH2	1:F:160:ASP:HB3	1.82	0.94
1:B:62:GLN:O	1:B:65:GLU:HG2	1.68	0.92
1:A:5:ILE:HD13	1:A:222:ALA:HB2	1.52	0.90
1:F:89:ARG:HH21	1:F:160:ASP:HB3	1.37	0.89
1:C:298:ILE:HG22	4:C:510:HOH:O	1.72	0.88
1:C:91:ASP:OD2	1:C:96:ARG:NH1	2.07	0.87
1:D:4:THR:HG23	1:D:7:SER:H	1.39	0.87
1:F:4:THR:HG23	1:F:7:SER:H	1.40	0.86
1:E:16:LEU:HB3	1:E:311:GLU:OE2	1.76	0.85
1:C:20:VAL:O	1:C:24:THR:HG23	1.77	0.84
1:E:5:ILE:HD13	1:E:222:ALA:HB2	1.56	0.84
1:F:177:VAL:HG22	1:F:178:PRO:HD2	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:191:GLU:OE1	1:F:254:ARG:NH1	2.10	0.84
1:C:187:LYS:HZ1	1:C:199:LEU:HB3	1.40	0.83
1:D:261:GLU:HG3	4:D:506:HOH:O	1.76	0.83
1:B:170:LYS:HE3	1:B:172:ILE:HD11	1.63	0.80
1:F:78:GLN:HB2	4:F:530:HOH:O	1.79	0.80
1:A:91:ASP:HB2	1:A:163:PHE:CE1	2.16	0.79
1:C:24:THR:HG22	4:C:523:HOH:O	1.81	0.79
1:C:16:LEU:HB3	1:C:311:GLU:OE2	1.85	0.76
1:E:77:LEU:HB3	1:E:78:GLN:OE1	1.87	0.74
1:A:247:ASN:O	1:A:276:PRO:HG3	1.89	0.73
1:C:127:ALA:HA	2:C:402:GOL:H31	1.69	0.73
1:C:89:ARG:HH21	1:C:160:ASP:HB3	1.54	0.73
1:A:308:SER:OG	1:C:310:LYS:HE2	1.89	0.72
1:E:9:ARG:HD2	1:E:224:GLN:OE1	1.89	0.72
1:A:9:ARG:HH11	1:A:9:ARG:HG2	1.54	0.71
1:A:66:ASN:OD1	4:A:501:HOH:O	2.09	0.70
1:F:78:GLN:OE1	1:F:81:GLN:HB3	1.92	0.69
1:E:293:ASN:HD21	1:E:297:LYS:CE	2.06	0.69
1:B:77:LEU:H	1:B:77:LEU:HD23	1.59	0.68
1:B:170:LYS:CE	1:B:172:ILE:HD11	2.24	0.67
1:E:223:LEU:CD2	1:E:301:VAL:HG13	2.24	0.67
1:D:238:LEU:HD11	1:D:242:ARG:CZ	2.24	0.67
1:F:80:THR:HG22	4:F:534:HOH:O	1.95	0.66
1:F:177:VAL:CG2	1:F:178:PRO:HD2	2.26	0.65
1:A:5:ILE:HD13	1:A:222:ALA:CB	2.26	0.65
1:B:91:ASP:HB2	1:B:163:PHE:CE2	2.31	0.65
1:C:187:LYS:HG2	1:C:203:ASP:OD2	1.97	0.65
1:F:134:ASN:O	1:F:138:VAL:HG23	1.96	0.65
1:A:56:PRO:HA	2:A:401:GOL:H32	1.79	0.65
1:C:77:LEU:HB3	1:C:78:GLN:NE2	2.11	0.65
1:A:5:ILE:CD1	1:A:222:ALA:HB2	2.26	0.64
1:F:146:GLU:HB2	4:F:504:HOH:O	1.97	0.64
1:E:223:LEU:HD22	1:E:301:VAL:HG13	1.80	0.63
1:A:117:MET:HE2	4:A:517:HOH:O	1.98	0.63
1:C:89:ARG:NH2	1:C:160:ASP:HB3	2.13	0.62
1:E:223:LEU:HD21	1:E:303:ILE:HD11	1.82	0.62
1:B:238:LEU:HD21	1:B:242:ARG:NE	2.13	0.62
1:F:4:THR:CG2	1:F:7:SER:HB3	2.29	0.62
1:C:169:GLY:HA2	4:C:532:HOH:O	1.99	0.62
1:D:114:GLY:O	1:D:118:GLU:HG3	2.00	0.62
1:A:16:LEU:N	1:A:311:GLU:OE1	2.28	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:236:ASN:OD1	1:E:239:ARG:NH2	2.32	0.61
1:C:128:GLY:H	2:C:402:GOL:C3	2.13	0.61
1:F:117:MET:HE2	4:F:521:HOH:O	2.01	0.61
1:A:154:LEU:O	1:A:158:VAL:HG13	2.00	0.60
1:E:5:ILE:CD1	1:E:222:ALA:HB2	2.29	0.60
1:B:177:VAL:CG2	1:B:178:PRO:HD2	2.30	0.60
1:C:16:LEU:CB	1:C:311:GLU:OE2	2.49	0.60
1:A:65:GLU:HG3	1:A:66:ASN:N	2.16	0.60
1:F:310:LYS:HB3	4:F:526:HOH:O	2.00	0.60
1:E:177:VAL:HG22	1:E:178:PRO:HD2	1.84	0.59
1:E:177:VAL:HG12	1:E:246:GLN:OE1	2.02	0.59
1:E:114:GLY:O	1:E:118:GLU:HG3	2.02	0.59
1:A:310:LYS:HE3	1:C:308:SER:OG	2.03	0.59
1:D:238:LEU:HD13	1:D:242:ARG:HD2	1.85	0.59
1:E:53:ILE:HG12	1:E:278:PHE:CE1	2.38	0.59
1:C:187:LYS:HD3	1:C:188:VAL:O	2.01	0.59
1:E:210:PHE:CD1	1:E:241:PHE:HB3	2.37	0.59
1:C:170:LYS:HA	4:C:532:HOH:O	2.03	0.58
1:A:92:THR:HB	1:A:93:PRO:HD2	1.85	0.58
1:C:218:THR:HG23	1:C:297:LYS:HB3	1.85	0.58
1:E:177:VAL:CG2	1:E:178:PRO:HD2	2.33	0.58
1:D:272:LYS:NZ	1:D:285:ASN:OD1	2.36	0.58
1:F:4:THR:HG22	1:F:7:SER:HB3	1.86	0.58
1:C:5:ILE:HD12	1:C:222:ALA:HB3	1.85	0.57
1:E:293:ASN:HD21	1:E:297:LYS:HE2	1.68	0.57
1:E:56:PRO:HA	2:E:401:GOL:H12	1.85	0.57
1:B:177:VAL:HG22	1:B:178:PRO:HD2	1.86	0.57
1:F:91:ASP:OD1	1:F:96:ARG:NE	2.38	0.57
1:C:210:PHE:CD1	1:C:241:PHE:HB3	2.38	0.57
1:A:215:GLU:O	1:A:297:LYS:NZ	2.23	0.57
1:D:238:LEU:CD1	1:D:242:ARG:HD2	2.35	0.57
1:B:210:PHE:CD1	1:B:241:PHE:HB3	2.40	0.56
1:C:62:GLN:O	1:C:65:GLU:HG2	2.05	0.56
1:A:114:GLY:O	1:A:118:GLU:HG3	2.04	0.56
1:B:114:GLY:O	1:B:118:GLU:HG3	2.05	0.56
1:C:39:LEU:C	1:C:39:LEU:HD23	2.26	0.56
1:D:238:LEU:HD11	1:D:242:ARG:NE	2.20	0.56
1:B:39:LEU:C	1:B:39:LEU:HD23	2.26	0.56
1:D:39:LEU:HD23	1:D:39:LEU:C	2.26	0.56
1:B:77:LEU:H	1:B:77:LEU:CD2	2.19	0.55
1:A:210:PHE:CD1	1:A:241:PHE:HB3	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:228:GLN:OE1	4:F:501:HOH:O	2.18	0.55
1:A:9:ARG:NH1	1:A:224:GLN:OE1	2.38	0.55
1:F:91:ASP:HB2	1:F:163:PHE:CE2	2.42	0.55
1:A:62:GLN:O	1:A:65:GLU:HG2	2.08	0.54
1:E:5:ILE:HD13	1:E:222:ALA:CB	2.32	0.54
1:B:238:LEU:HD21	1:B:242:ARG:CZ	2.38	0.54
1:F:89:ARG:NH2	1:F:160:ASP:CB	2.65	0.54
1:C:114:GLY:O	1:C:118:GLU:HG3	2.08	0.54
1:E:103:PRO:O	1:E:107:LEU:HD22	2.07	0.53
1:F:80:THR:CG2	4:F:534:HOH:O	2.55	0.53
1:D:171:ARG:NH1	1:D:243:GLU:OE1	2.41	0.53
1:E:170:LYS:O	1:E:171:ARG:HG3	2.08	0.53
1:B:27:ARG:O	4:B:501:HOH:O	2.19	0.53
1:B:14:ASN:OD1	1:F:133:ALA:N	2.42	0.53
1:C:63:LEU:HD23	1:C:105:ILE:HD11	1.91	0.53
1:B:77:LEU:N	1:B:77:LEU:HD23	2.23	0.53
1:F:39:LEU:HD23	1:F:39:LEU:C	2.29	0.53
1:B:238:LEU:CD2	1:B:242:ARG:HD2	2.40	0.52
1:A:9:ARG:NH1	1:A:9:ARG:HG2	2.23	0.52
1:D:191:GLU:HB2	1:D:254:ARG:HG2	1.91	0.52
1:E:223:LEU:C	1:E:223:LEU:HD13	2.30	0.52
1:C:16:LEU:O	1:C:311:GLU:OE1	2.28	0.52
1:C:177:VAL:HG22	1:C:246:GLN:OE1	2.10	0.52
1:E:223:LEU:HD23	1:E:301:VAL:CG1	2.39	0.52
1:E:295:GLU:OE1	1:E:297:LYS:HE2	2.10	0.52
1:E:289:ARG:O	1:E:301:VAL:HA	2.10	0.52
1:E:223:LEU:HD23	1:E:301:VAL:HG13	1.92	0.52
1:B:5:ILE:HD12	1:B:222:ALA:HB3	1.93	0.51
1:A:310:LYS:HE3	1:C:308:SER:CB	2.41	0.51
1:C:223:LEU:HD23	1:C:223:LEU:C	2.31	0.51
1:E:113:LEU:O	1:E:117:MET:HE2	2.10	0.51
1:F:49:LYS:NZ	4:F:507:HOH:O	2.35	0.51
1:C:187:LYS:NZ	1:C:199:LEU:HB3	2.20	0.51
1:A:132:SER:HB2	1:B:13:PRO:O	2.11	0.50
1:B:311:GLU:OE1	1:B:311:GLU:N	2.44	0.50
1:F:5:ILE:HD12	1:F:222:ALA:HB3	1.93	0.50
1:E:39:LEU:HD23	1:E:39:LEU:C	2.31	0.50
1:C:14:ASN:HB3	4:C:541:HOH:O	2.12	0.49
1:A:16:LEU:HB3	1:A:311:GLU:CD	2.32	0.49
1:A:39:LEU:C	1:A:39:LEU:HD23	2.33	0.49
1:D:91:ASP:HB2	1:D:163:PHE:CE2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:62:GLN:O	1:F:65:GLU:HG2	2.12	0.49
1:E:103:PRO:O	1:E:107:LEU:CD2	2.60	0.49
1:A:107:LEU:HD23	1:A:158:VAL:HG21	1.93	0.49
1:A:53:ILE:HD13	1:A:111:TYR:HD1	1.77	0.49
1:B:53:ILE:HD13	1:B:111:TYR:HD2	1.78	0.49
1:A:100:SER:HB2	1:A:170:LYS:O	2.12	0.49
1:B:238:LEU:HD23	1:B:242:ARG:HD2	1.95	0.48
1:D:4:THR:CG2	1:D:7:SER:HB3	2.43	0.48
1:A:47:MET:HE3	1:A:51:LEU:HD12	1.95	0.48
1:B:89:ARG:HA	1:B:162:GLY:O	2.14	0.48
1:C:3:PHE:CZ	1:C:261:GLU:HB2	2.49	0.48
1:C:91:ASP:HB2	1:C:163:PHE:CE1	2.49	0.47
1:D:223:LEU:C	1:D:223:LEU:HD23	2.35	0.47
1:E:110:TRP:HB3	3:E:402:EQ3:C7	2.44	0.47
1:E:18:ALA:HB2	1:E:307:ALA:HA	1.95	0.47
1:A:18:ALA:HB2	1:A:307:ALA:HA	1.96	0.47
1:B:3:PHE:CE2	1:B:291:LEU:HD21	2.47	0.47
1:F:114:GLY:O	1:F:118:GLU:HG3	2.14	0.47
1:C:75:GLY:O	1:C:79:GLN:HG3	2.14	0.47
1:C:134:ASN:O	1:C:138:VAL:HG23	2.14	0.47
1:C:65:GLU:HG3	1:C:66:ASN:N	2.29	0.47
1:C:132:SER:HB2	1:D:13:PRO:O	2.15	0.47
1:F:41:TRP:CZ2	1:F:45:LEU:HD11	2.50	0.47
1:A:191:GLU:HB2	1:A:254:ARG:HG2	1.97	0.47
1:B:77:LEU:HD21	1:B:78:GLN:OE1	2.15	0.47
1:D:238:LEU:C	1:D:238:LEU:HD13	2.35	0.47
1:A:99:ALA:HB2	1:A:163:PHE:H	1.80	0.47
1:C:128:GLY:N	2:C:402:GOL:O3	2.38	0.47
1:A:110:TRP:HB3	3:A:402:EQ3:C7	2.45	0.47
1:E:3:PHE:CE2	1:E:261:GLU:HB2	2.51	0.46
1:E:75:GLY:O	1:E:79:GLN:HG3	2.15	0.46
1:F:187:LYS:HE3	4:F:522:HOH:O	2.14	0.46
1:A:170:LYS:HD2	1:A:170:LYS:O	2.14	0.46
1:B:238:LEU:HD23	1:B:238:LEU:C	2.35	0.46
1:C:254:ARG:NH1	1:C:254:ARG:HB3	2.30	0.46
1:B:91:ASP:HB2	1:B:163:PHE:CD2	2.51	0.46
1:C:131:LEU:HB3	1:C:135:ALA:HB3	1.98	0.46
1:A:289:ARG:O	1:A:301:VAL:HA	2.16	0.46
1:C:273:VAL:HG12	1:C:274:GLN:N	2.31	0.46
1:E:16:LEU:HB3	1:E:311:GLU:CD	2.36	0.46
1:C:76:PRO:HD2	4:C:530:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:272:LYS:HA	1:F:284:MET:O	2.14	0.46
1:C:187:LYS:HD3	1:C:188:VAL:N	2.31	0.46
1:F:229:ARG:HG2	4:F:528:HOH:O	2.16	0.46
1:B:110:TRP:HB3	3:B:401:EQ3:C7	2.46	0.45
1:D:32:ASN:HB3	1:D:35:ASP:OD2	2.17	0.45
1:E:22:PRO:HG3	1:E:227:PHE:CD1	2.51	0.45
1:B:66:ASN:O	1:B:70[B]:GLU:HG3	2.16	0.45
1:C:104:ASN:HB2	1:C:174:GLU:OE2	2.16	0.45
1:C:40:ILE:HG21	3:C:403:EQ3:C5	2.46	0.45
1:F:41:TRP:CE2	1:F:45:LEU:HD11	2.52	0.45
1:A:223:LEU:C	1:A:223:LEU:HD23	2.37	0.45
1:A:71:ILE:O	1:A:79:GLN:HG2	2.17	0.45
1:D:134:ASN:O	1:D:138:VAL:HG23	2.17	0.45
1:F:22:PRO:HG3	1:F:227:PHE:CD1	2.52	0.45
1:D:28:PHE:CE2	1:D:157:ALA:HB1	2.52	0.45
1:F:146:GLU:N	4:F:504:HOH:O	2.27	0.45
1:F:21:VAL:HB	1:F:22:PRO:CD	2.47	0.44
1:D:272:LYS:HA	1:D:284:MET:O	2.17	0.44
1:F:75:GLY:O	1:F:79:GLN:HG3	2.17	0.44
1:A:28:PHE:CZ	1:A:36:GLN:HB3	2.52	0.44
1:C:110:TRP:HB3	3:C:403:EQ3:C7	2.47	0.44
1:F:124:PRO:HB2	4:F:521:HOH:O	2.17	0.44
1:E:13:PRO:O	1:F:132:SER:HB2	2.18	0.44
1:F:223:LEU:HD23	1:F:223:LEU:C	2.38	0.44
1:F:62:GLN:HA	1:F:62:GLN:OE1	2.18	0.44
1:C:163:PHE:HA	1:C:164:THR:HA	1.79	0.44
1:C:289:ARG:O	1:C:301:VAL:HA	2.18	0.44
1:C:44:TYR:HE1	1:C:53:ILE:CD1	2.31	0.44
1:C:41:TRP:CZ2	1:C:45:LEU:HD11	2.52	0.44
1:D:112:ARG:NH1	1:D:115:GLU:OE1	2.50	0.44
1:A:23:ALA:HB1	1:B:23:ALA:HB1	1.99	0.44
1:C:275:THR:OG1	1:C:276:PRO:HD2	2.18	0.44
1:C:225:PRO:HD2	1:C:228:GLN:HB2	1.99	0.43
1:E:172:ILE:HD12	1:E:172:ILE:N	2.33	0.43
1:F:210:PHE:CD1	1:F:241:PHE:HB3	2.53	0.43
1:B:81:GLN:NE2	1:B:85:ASP:OD1	2.50	0.43
1:D:110:TRP:HB3	3:D:401:EQ3:C7	2.48	0.43
1:E:223:LEU:HD13	1:E:224:GLN:N	2.32	0.43
1:C:174:GLU:HG3	1:C:174:GLU:H	1.67	0.43
1:E:208:ASN:OD1	1:E:246:GLN:HA	2.18	0.43
1:D:89:ARG:HA	1:D:162:GLY:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:310:LYS:HB3	4:E:515:HOH:O	2.19	0.43
1:C:254:ARG:HH11	1:C:254:ARG:HB3	1.84	0.43
1:E:23:ALA:HB1	1:F:23:ALA:HB1	2.01	0.43
1:E:223:LEU:CD2	1:E:303:ILE:HD11	2.46	0.43
1:C:56:PRO:HA	2:C:401:GOL:H11	2.00	0.43
1:E:257:THR:HG23	1:E:267:ILE:HG12	2.01	0.43
1:E:272:LYS:HA	1:E:284:MET:O	2.18	0.43
1:E:40:ILE:HG21	3:E:402:EQ3:C5	2.48	0.43
1:D:247:ASN:HB2	1:D:276:PRO:HG3	2.01	0.43
1:E:134:ASN:O	1:E:138:VAL:HG23	2.19	0.43
1:A:134:ASN:O	1:A:138:VAL:HG23	2.19	0.42
1:D:311:GLU:OE1	1:D:311:GLU:N	2.52	0.42
1:E:132:SER:HB2	1:F:13:PRO:O	2.19	0.42
1:E:293:ASN:HD21	1:E:297:LYS:HE3	1.79	0.42
1:B:19:ASP:HA	1:B:22:PRO:HD2	2.00	0.42
1:D:104:ASN:O	4:D:501:HOH:O	2.21	0.42
1:D:26:ALA:O	1:D:30:GLN:HG2	2.20	0.42
1:D:75:GLY:O	1:D:79:GLN:HG3	2.18	0.42
1:A:170:LYS:H	1:A:170:LYS:HG3	1.71	0.42
1:C:117:MET:HB3	1:C:117:MET:HE2	1.83	0.42
1:E:214:ILE:HD12	1:E:214:ILE:HA	1.91	0.42
1:A:77:LEU:HB2	1:A:78:GLN:HE22	1.84	0.42
1:E:21:VAL:HB	1:E:22:PRO:CD	2.49	0.42
1:A:247:ASN:HB2	1:A:276:PRO:CG	2.50	0.42
1:A:181:ASP:OD1	1:A:184:SER:OG	2.29	0.42
1:B:89:ARG:HB3	1:B:162:GLY:O	2.19	0.41
1:B:177:VAL:HG23	1:B:178:PRO:HD2	2.02	0.41
1:B:77:LEU:CD2	1:B:78:GLN:OE1	2.68	0.41
1:B:130:GLN:HA	4:C:519:HOH:O	2.20	0.41
1:E:125:ILE:HA	1:E:125:ILE:HD13	1.76	0.41
1:B:41:TRP:CE2	1:B:45:LEU:HD11	2.56	0.41
1:C:13:PRO:O	1:D:132:SER:HB2	2.21	0.41
1:C:301:VAL:HG13	1:C:301:VAL:O	2.20	0.41
1:A:310:LYS:CE	1:C:308:SER:CB	2.98	0.41
1:E:28:PHE:CZ	1:E:40:ILE:HD11	2.55	0.41
1:E:28:PHE:CE2	1:E:157:ALA:HB1	2.55	0.41
1:E:59:ALA:HB3	4:E:508:HOH:O	2.20	0.41
1:E:78:GLN:N	1:E:78:GLN:OE1	2.54	0.41
1:D:2:PRO:O	1:D:3:PHE:CB	2.69	0.41
1:A:75:GLY:O	1:A:79:GLN:HG3	2.20	0.41
1:E:293:ASN:ND2	1:E:297:LYS:HG3	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:89:ARG:NE	1:F:160:ASP:O	2.54	0.41
1:F:214:ILE:HD12	1:F:214:ILE:HA	1.89	0.41
1:B:272:LYS:HA	1:B:284:MET:O	2.21	0.41
1:C:131:LEU:HB2	1:C:136:ASN:OD1	2.20	0.41
1:A:214:ILE:HD12	1:A:214:ILE:HA	1.93	0.41
1:D:5:ILE:HA	1:D:5:ILE:HD13	1.98	0.41
1:E:301:VAL:O	1:E:301:VAL:HG13	2.21	0.41
1:E:49:LYS:NZ	4:E:501:HOH:O	2.23	0.40
1:F:289:ARG:O	1:F:301:VAL:HA	2.21	0.40
1:C:163:PHE:C	1:C:163:PHE:CD2	2.94	0.40
1:C:218:THR:CG2	1:C:297:LYS:HB3	2.50	0.40
1:A:91:ASP:HB2	1:A:163:PHE:CD1	2.55	0.40
1:C:78:GLN:CD	1:C:78:GLN:H	2.24	0.40
1:D:303:ILE:N	1:D:303:ILE:HD12	2.36	0.40
1:E:91:ASP:HB2	1:E:163:PHE:CE1	2.56	0.40
1:A:77:LEU:HB2	1:A:78:GLN:NE2	2.36	0.40
1:B:134:ASN:O	1:B:138:VAL:HG23	2.21	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	303/323 (94%)	301 (99%)	2 (1%)	0	100	100
1	B	303/323 (94%)	301 (99%)	2 (1%)	0	100	100
1	C	303/323 (94%)	300 (99%)	3 (1%)	0	100	100
1	D	305/323 (94%)	301 (99%)	3 (1%)	1 (0%)	44	55
1	E	303/323 (94%)	299 (99%)	3 (1%)	1 (0%)	44	55
1	F	303/323 (94%)	301 (99%)	2 (1%)	0	100	100
All	All	1820/1938 (94%)	1803 (99%)	15 (1%)	2 (0%)	55	67

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	3	PHE
1	E	170	LYS

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	250/263 (95%)	244 (98%)	6 (2%)	54	72
1	B	251/263 (95%)	245 (98%)	6 (2%)	54	72
1	C	250/263 (95%)	246 (98%)	4 (2%)	68	82
1	D	251/263 (95%)	249 (99%)	2 (1%)	85	93
1	E	250/263 (95%)	246 (98%)	4 (2%)	68	82
1	F	250/263 (95%)	247 (99%)	3 (1%)	75	87
All	All	1502/1578 (95%)	1477 (98%)	25 (2%)	66	81

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	ILE
1	A	77	LEU
1	A	170	LYS
1	A	182	THR
1	A	304	ASP
1	A	310	LYS
1	B	3	PHE
1	B	4	THR
1	B	78	GLN
1	B	136	ASN
1	B	182	THR
1	B	254	ARG
1	C	63	LEU
1	C	136	ASN
1	C	182	THR

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Mol	Chain	Res	Type
1	C	254	ARG
1	D	3	PHE
1	D	182	THR
1	E	78	GLN
1	E	182	THR
1	E	229	ARG
1	E	239	ARG
1	F	78	GLN
1	F	80	THR
1	F	182	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	GLN
1	C	78	GLN

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](#)

10 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	GOL	A	401	-	5,5,5	0.39	0	5,5,5	0.76	0
3	EQ3	A	402	-	43,43,43	0.85	0	55,60,60	1.31	10 (18%)
3	EQ3	B	401	-	43,43,43	0.84	0	55,60,60	1.31	5 (9%)
2	GOL	C	401	-	5,5,5	0.30	0	5,5,5	0.67	0
2	GOL	C	402	-	5,5,5	0.28	0	5,5,5	0.74	0
3	EQ3	C	403	-	43,43,43	0.85	0	55,60,60	1.34	8 (14%)
3	EQ3	D	401	-	43,43,43	0.83	0	55,60,60	1.35	7 (12%)
2	GOL	E	401	-	5,5,5	0.38	0	5,5,5	0.60	0
3	EQ3	E	402	-	43,43,43	0.88	1 (2%)	55,60,60	1.36	7 (12%)
3	EQ3	F	401	-	43,43,43	0.86	0	55,60,60	1.34	7 (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	GOL	A	401	-	-	0/4/4/4	0/0/0/0
3	EQ3	A	402	-	-	0/29/68/68	0/2/2/2
3	EQ3	B	401	-	-	0/29/68/68	0/2/2/2
2	GOL	C	401	-	-	0/4/4/4	0/0/0/0
2	GOL	C	402	-	-	0/4/4/4	0/0/0/0
3	EQ3	C	403	-	-	0/29/68/68	0/2/2/2
3	EQ3	D	401	-	-	0/29/68/68	0/2/2/2
2	GOL	E	401	-	-	0/4/4/4	0/0/0/0
3	EQ3	E	402	-	-	0/29/68/68	0/2/2/2
3	EQ3	F	401	-	-	0/29/68/68	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	402	EQ3	C8-C9	2.22	1.50	1.45

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	401	EQ3	C16-C17-C18	-4.12	121.44	127.31
3	D	401	EQ3	C16-C17-C18	-3.95	121.67	127.31
3	B	401	EQ3	C20-C21-C22	-3.61	122.16	127.31
3	C	403	EQ3	C16-C17-C18	-3.60	122.17	127.31
3	E	402	EQ3	C24-C23-C22	-3.53	120.91	126.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	EQ3	C20-C21-C22	-3.37	122.50	127.31
3	B	401	EQ3	C16-C17-C18	-3.31	122.58	127.31
3	E	402	EQ3	C20-C21-C22	-3.23	122.70	127.31
3	F	401	EQ3	C20-C21-C22	-3.16	122.80	127.31
3	C	403	EQ3	C20-C21-C22	-3.14	122.83	127.31
3	E	402	EQ3	C16-C17-C18	-2.95	123.09	127.31
3	A	402	EQ3	C24-C23-C22	-2.92	121.82	126.21
3	C	403	EQ3	C24-C23-C22	-2.92	121.82	126.21
3	D	401	EQ3	C20-C21-C22	-2.83	123.27	127.31
3	D	401	EQ3	C36-C18-C17	-2.69	119.15	122.92
3	F	401	EQ3	C38-C26-C25	-2.69	120.30	123.92
3	B	401	EQ3	C38-C26-C25	-2.68	120.31	123.92
3	A	402	EQ3	C16-C17-C18	-2.64	123.54	127.31
3	D	401	EQ3	C7-C8-C9	-2.62	122.27	126.21
3	A	402	EQ3	C7-C8-C9	-2.59	122.32	126.21
3	C	403	EQ3	C7-C8-C9	-2.57	122.35	126.21
3	C	403	EQ3	C33-C5-C6	-2.46	121.75	124.51
3	B	401	EQ3	C7-C8-C9	-2.44	122.55	126.21
3	A	402	EQ3	C33-C5-C6	-2.35	121.88	124.51
3	F	401	EQ3	C15-C14-C13	-2.34	123.97	127.31
3	A	402	EQ3	C15-C14-C13	-2.33	123.98	127.31
3	B	401	EQ3	C23-C24-C25	-2.32	120.76	127.25
3	D	401	EQ3	C23-C24-C25	-2.30	120.80	127.25
3	D	401	EQ3	C15-C14-C13	-2.28	124.06	127.31
3	C	403	EQ3	C11-C10-C9	-2.27	124.07	127.31
3	F	401	EQ3	C36-C18-C17	-2.26	119.75	122.92
3	C	403	EQ3	C37-C22-C21	-2.25	119.77	122.92
3	F	401	EQ3	C24-C23-C22	-2.25	122.83	126.21
3	E	402	EQ3	C29-C28-C27	-2.23	108.73	112.80
3	F	401	EQ3	C37-C22-C21	-2.19	119.85	122.92
3	E	402	EQ3	C38-C26-C25	-2.16	121.01	123.92
3	A	402	EQ3	C38-C26-C25	-2.14	121.04	123.92
3	A	402	EQ3	C11-C10-C9	-2.10	124.31	127.31
3	C	403	EQ3	C15-C14-C13	-2.08	124.34	127.31
3	E	402	EQ3	C7-C8-C9	-2.04	123.15	126.21
3	A	402	EQ3	C36-C18-C17	-2.02	120.09	122.92
3	E	402	EQ3	C23-C24-C25	-2.01	121.62	127.25
3	A	402	EQ3	C40-C30-C25	2.08	113.69	110.31
3	D	401	EQ3	C37-C22-C23	2.27	121.72	118.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	GOL	1	0
3	A	402	EQ3	1	0
3	B	401	EQ3	1	0
2	C	401	GOL	1	0
2	C	402	GOL	3	0
3	C	403	EQ3	2	0
3	D	401	EQ3	1	0
2	E	401	GOL	1	0
3	E	402	EQ3	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	305/323 (94%)	0.42	13 (4%) 36 43	29, 53, 86, 116	0
1	B	304/323 (94%)	0.33	15 (4%) 30 37	30, 54, 84, 122	0
1	C	305/323 (94%)	0.50	20 (6%) 19 25	28, 53, 87, 120	0
1	D	306/323 (94%)	0.45	10 (3%) 47 54	28, 54, 84, 120	0
1	E	305/323 (94%)	0.42	16 (5%) 28 35	27, 54, 87, 125	0
1	F	305/323 (94%)	0.47	13 (4%) 36 43	30, 53, 86, 109	0
All	All	1830/1938 (94%)	0.43	87 (4%) 31 38	27, 53, 87, 125	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	311	GLU	12.0
1	A	309	PRO	10.0
1	C	311	GLU	6.5
1	C	3	PHE	6.0
1	C	308	SER	5.8
1	A	3	PHE	5.6
1	A	51	LEU	5.3
1	E	309	PRO	5.2
1	E	217	PHE	4.8
1	E	163	PHE	4.4
1	C	309	PRO	4.3
1	C	52	THR	4.2
1	C	51	LEU	3.9
1	F	103	PRO	3.8
1	E	47	MET	3.7
1	B	311	GLU	3.6
1	A	176	VAL	3.6
1	F	47	MET	3.6
1	D	262	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	183	ALA	3.5
1	D	55	ALA	3.5
1	A	44	TYR	3.4
1	B	154	LEU	3.4
1	B	309	PRO	3.3
1	E	164	THR	3.3
1	F	311	GLU	3.2
1	B	175	PRO	3.0
1	D	51	LEU	3.0
1	D	3	PHE	3.0
1	A	170	LYS	3.0
1	D	47	MET	2.9
1	B	53	ILE	2.7
1	C	199	LEU	2.7
1	B	164	THR	2.7
1	E	210	PHE	2.7
1	F	282	VAL	2.7
1	F	71	ILE	2.6
1	D	53	ILE	2.6
1	B	245	CYS	2.6
1	F	309	PRO	2.6
1	A	248	LEU	2.5
1	C	163	PHE	2.5
1	E	110	TRP	2.5
1	D	123	ALA	2.5
1	F	240	PHE	2.4
1	E	310	LYS	2.4
1	C	53	ILE	2.4
1	F	172	ILE	2.4
1	A	38	ALA	2.4
1	A	187	LYS	2.4
1	F	238	LEU	2.4
1	B	24	THR	2.4
1	F	173	ALA	2.3
1	E	70[A]	GLU	2.3
1	B	44	TYR	2.3
1	A	5	ILE	2.3
1	E	125	ILE	2.3
1	C	50	THR	2.3
1	C	261	GLU	2.3
1	C	237	VAL	2.3
1	C	126	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	176	VAL	2.2
1	D	275	THR	2.2
1	E	174	GLU	2.2
1	C	33	ALA	2.2
1	F	135	ALA	2.2
1	E	65	GLU	2.2
1	C	68	LEU	2.2
1	B	188	VAL	2.2
1	F	264	PHE	2.2
1	A	172	ILE	2.2
1	B	40	ILE	2.2
1	C	238	LEU	2.2
1	C	240	PHE	2.1
1	B	49	LYS	2.1
1	D	42	PHE	2.1
1	B	94	LEU	2.1
1	B	3	PHE	2.1
1	E	187	LYS	2.1
1	E	299	PHE	2.1
1	A	154	LEU	2.1
1	F	164	THR	2.1
1	C	157	ALA	2.1
1	E	76	PRO	2.1
1	C	25	ILE	2.0
1	A	125	ILE	2.0
1	D	205	LEU	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	EQ3	E	402	42/42	0.85	0.42	5.81	35,57,75,80	0
3	EQ3	C	403	42/42	0.86	0.36	4.52	33,58,74,77	0
3	EQ3	F	401	42/42	0.90	0.36	4.32	39,54,69,74	0
3	EQ3	A	402	42/42	0.86	0.36	3.96	36,57,71,79	0
3	EQ3	D	401	42/42	0.84	0.33	3.92	37,58,72,76	0
3	EQ3	B	401	42/42	0.84	0.35	3.43	41,59,76,78	0
2	GOL	C	401	6/6	0.80	0.26	1.44	64,83,94,106	0
2	GOL	A	401	6/6	0.79	0.17	1.09	62,75,87,87	0
2	GOL	E	401	6/6	0.76	0.15	-0.16	64,77,89,90	0
2	GOL	C	402	6/6	0.85	0.16	-0.43	66,81,98,99	0

6.5 Other polymers [i](#)

There are no such residues in this entry.