W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report (i)

Jun 20, 2016 – 06:52 AM EDT

PDB ID	:	5DQR
Title	:	The crystal structure of Arabidopsis 7-hydroxymethyl chlorophyll a reductase (HCAR)
Authors	:	Wang, X.; Liu, L.
Deposited on	:	2015-09-15
Resolution	:	2.70 Å(reported)

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

MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027790
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)	:	rb-20027790

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 2.70 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	Percentile Ranks	Value
Rfree		0.245
Clashscore		11
Ramachandran outliers		0.3%
Sidechain outliers		3.2%
RSRZ outliers		2.6%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
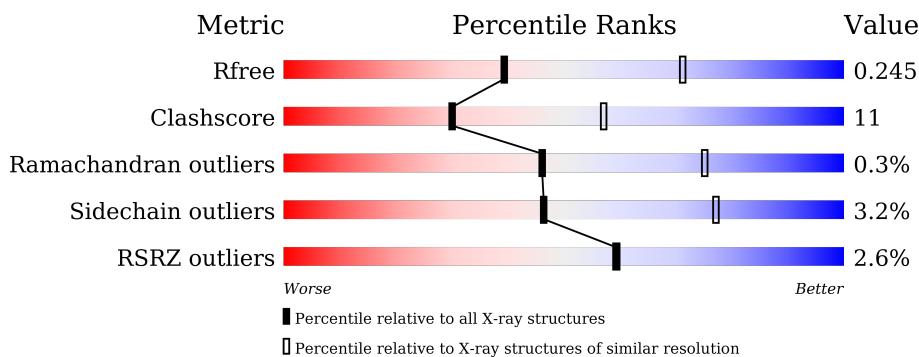
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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 <=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	437	5% / 73% / 20% / • 5%
1	B	437	2% / 73% / 19% / • 6%
1	C	437	% / 76% / 19% / • •
1	D	437	% / 73% / 19% / • 6%
1	E	437	73% / 18% / • 7%
1	F	437	5% / 76% / 18% / • 5%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 20316 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 7-hydroxymethyl chlorophyll a reductase, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	414	Total	C	N	O	S	0	1	0
			3227	2050	558	599	20			
1	B	411	Total	C	N	O	S	0	1	0
			3197	2033	548	596	20			
1	C	421	Total	C	N	O	S	0	1	0
			3294	2089	567	618	20			
1	D	411	Total	C	N	O	S	0	0	0
			3198	2032	550	596	20			
1	E	406	Total	C	N	O	S	0	0	0
			3150	2002	542	586	20			
1	F	413	Total	C	N	O	S	0	1	0
			3214	2043	551	600	20			

- Molecule 2 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).
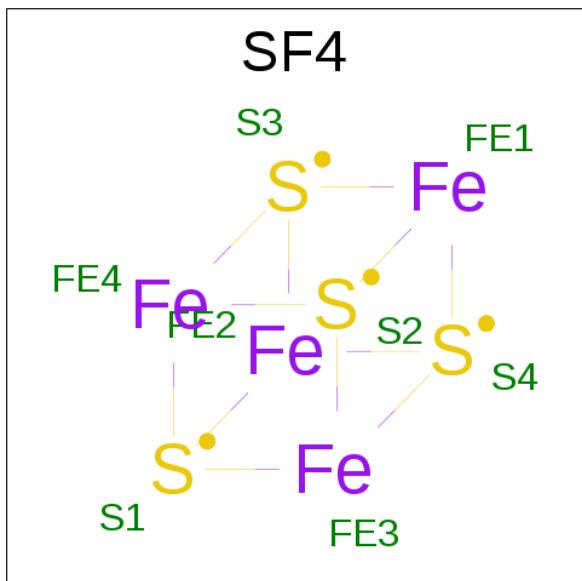
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 8	Fe 4	S 4	0	0
2	A	1	Total 8	Fe 4	S 4	0	0
2	B	1	Total 8	Fe 4	S 4	0	0
2	B	1	Total 8	Fe 4	S 4	0	0
2	C	1	Total 8	Fe 4	S 4	0	0
2	C	1	Total 8	Fe 4	S 4	0	0
2	D	1	Total 8	Fe 4	S 4	0	0
2	D	1	Total 8	Fe 4	S 4	0	0
2	E	1	Total 8	Fe 4	S 4	0	0
2	E	1	Total 8	Fe 4	S 4	0	0
2	F	1	Total 8	Fe 4	S 4	0	0
2	F	1	Total 8	Fe 4	S 4	0	0

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).
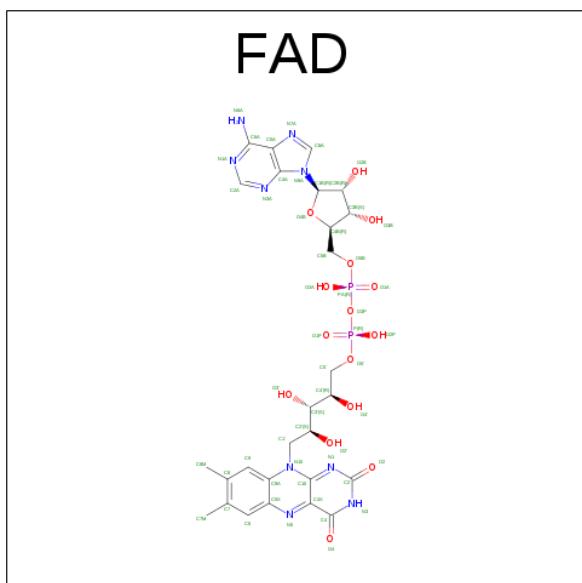
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
3	B	1	Total 53	C 27	N 9	O 15	P 2	0	0
3	C	1	Total 53	C 27	N 9	O 15	P 2	0	0
3	D	1	Total 53	C 27	N 9	O 15	P 2	0	0
3	E	1	Total 53	C 27	N 9	O 15	P 2	0	0
3	F	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	81	Total 81	O 81	0	0
4	B	118	Total 118	O 118	0	0
4	C	103	Total 103	O 103	0	0
4	D	151	Total 151	O 151	0	0
4	E	108	Total 108	O 108	0	0
4	F	61	Total 61	O 61	0	0

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: 7-hydroxymethyl chlorophyll a reductase, chloroplastic
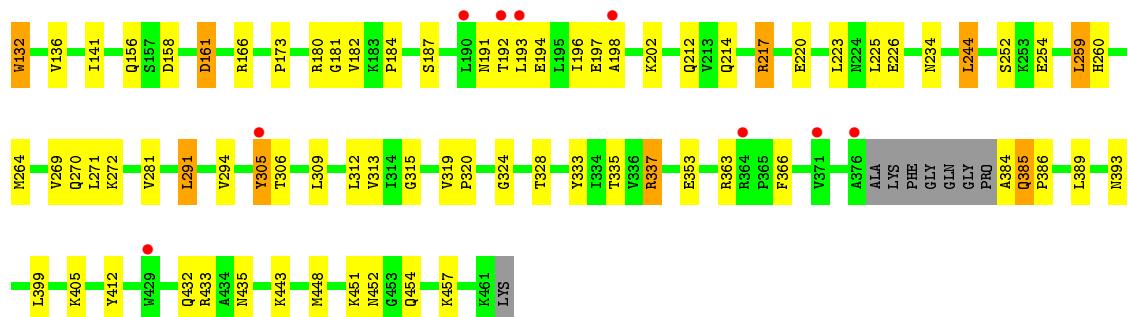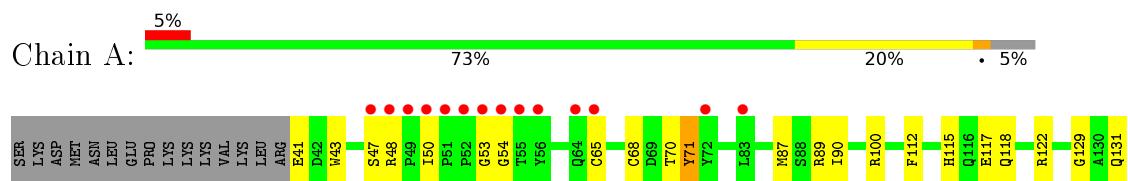

- Molecule 1: 7-hydroxymethyl chlorophyll a reductase, chloroplastic

- Molecule 1: 7-hydroxymethyl chlorophyll a reductase, chloroplastic

• Molecule 1: 7-hydroxymethyl chlorophyll a reductase, chloroplastic

Chain D:

• Molecule 1: 7-hydroxymethyl chlorophyll a reductase, chloroplastic

Chain E:

• Molecule 1: 7-hydroxymethyl chlorophyll a reductase, chloroplastic

Chain F:
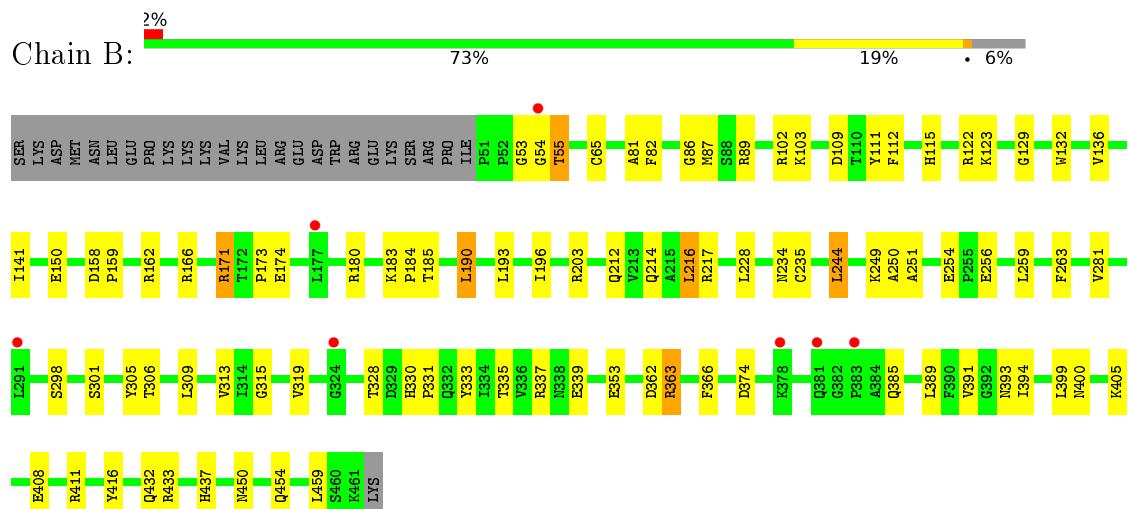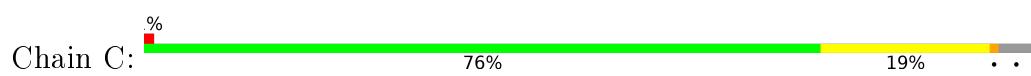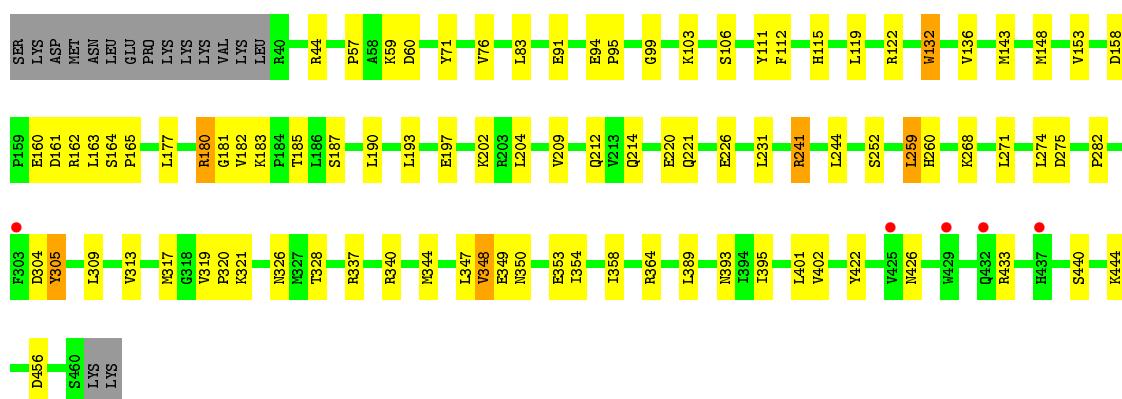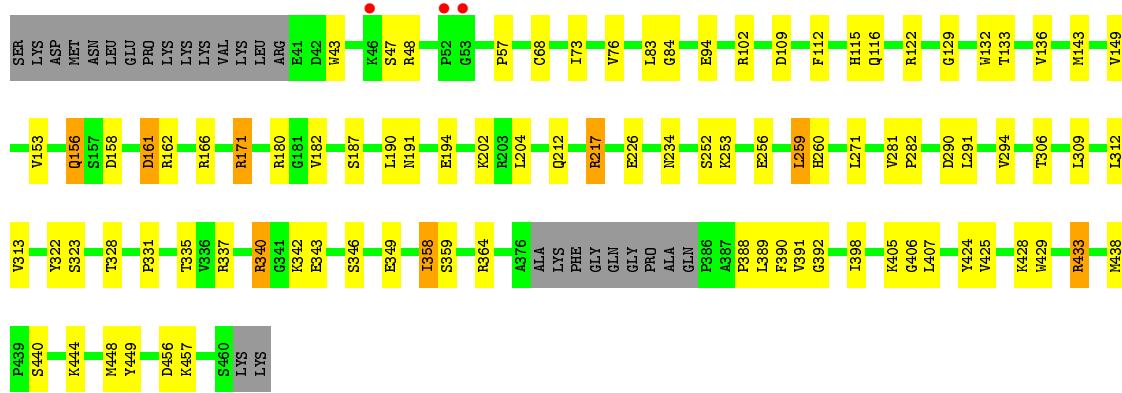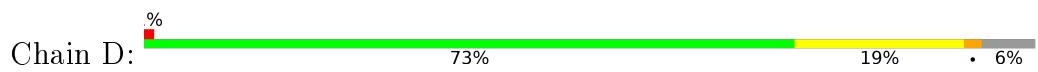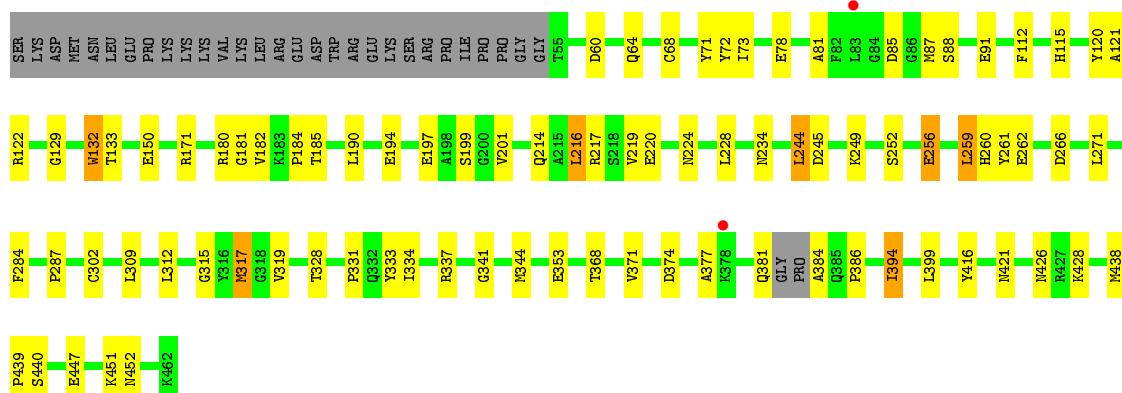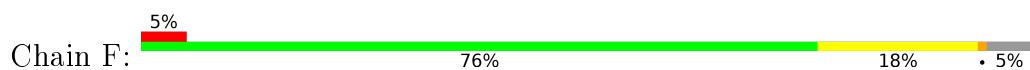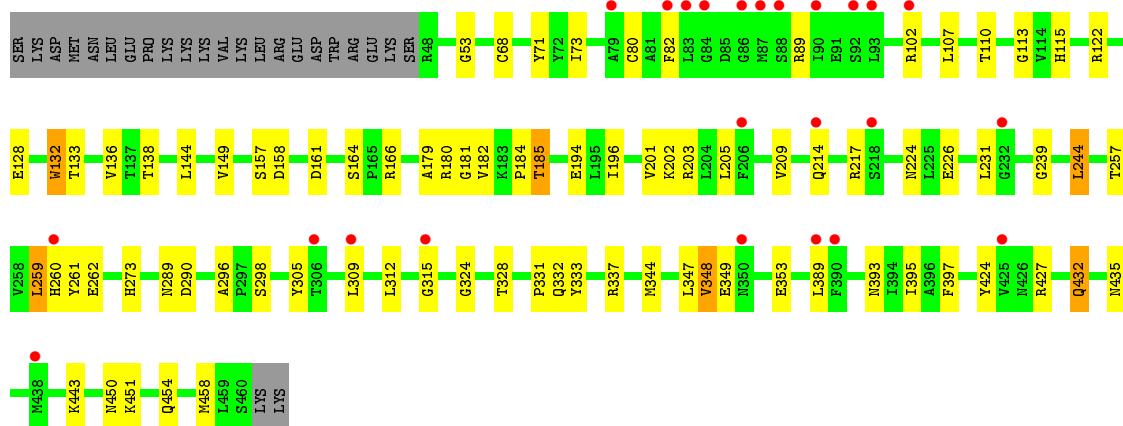
4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	89.11Å 89.11Å 273.31Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.61 – 2.70 44.61 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.7 (44.61-2.70) 97.8 (44.61-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	2.35 (at 2.69Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.202 , 0.246 0.201 , 0.245	Depositor DCC
R_{free} test set	3311 reflections (5.08%)	DCC
Wilson B-factor (Å^2)	39.6	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 25.0	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.010 for -h,-k,l 0.043 for h,-h-k,-l 0.058 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	20316	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.50% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: SF4, FAD

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	0.22	0/3300	0.45	3/4478 (0.1%)
1	B	0.22	0/3271	0.42	1/4437 (0.0%)
1	C	0.28	0/3370	0.55	4/4574 (0.1%)
1	D	0.21	0/3268	0.48	3/4436 (0.1%)
1	E	0.21	0/3216	0.45	3/4361 (0.1%)
1	F	0.26	0/3288	0.45	2/4464 (0.0%)
All	All	0.24	0/19713	0.47	16/26750 (0.1%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	348	VAL	CB-CA-C	-15.97	81.05	111.40
1	C	349	GLU	N-CA-CB	-10.82	91.12	110.60
1	C	348	VAL	N-CA-C	10.10	138.28	111.00
1	D	161	ASP	CB-CA-C	8.95	128.29	110.40
1	D	161	ASP	N-CA-C	-8.10	89.14	111.00
1	F	132	TRP	N-CA-C	7.19	130.42	111.00
1	E	132	TRP	N-CA-C	6.96	129.79	111.00
1	D	156	GLN	CB-CA-C	-6.63	97.14	110.40
1	A	132	TRP	N-CA-C	6.22	127.79	111.00
1	F	179	ALA	CB-CA-C	5.77	118.76	110.10
1	E	199	SER	CB-CA-C	5.58	120.70	110.10
1	C	132	TRP	N-CA-C	5.53	125.94	111.00
1	B	459	LEU	CB-CA-C	5.53	120.71	110.20
1	A	198	ALA	CB-CA-C	5.49	118.33	110.10
1	A	161	ASP	CB-CA-C	5.39	121.18	110.40
1	E	78	GLU	CB-CA-C	5.05	120.50	110.40

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	3227	0	3194	80	0
1	B	3197	0	3165	73	1
1	C	3294	0	3257	71	1
1	D	3198	0	3155	76	0
1	E	3150	0	3114	69	0
1	F	3214	0	3190	65	0
2	A	16	0	0	0	0
2	B	16	0	0	1	0
2	C	16	0	0	0	0
2	D	16	0	0	0	0
2	E	16	0	0	0	0
2	F	16	0	0	0	0
3	A	53	0	31	3	0
3	B	53	0	30	2	0
3	C	53	0	31	4	0
3	D	53	0	30	4	0
3	E	53	0	31	3	0
3	F	53	0	31	4	0
4	A	81	0	0	31	2
4	B	118	0	0	30	0
4	C	103	0	0	34	2
4	D	151	0	0	34	3
4	E	108	0	0	25	5
4	F	61	0	0	24	0
All	All	20316	0	19259	431	7

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 11.

All (431) 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:A:193:LEU:HG	4:A:613:HOH:O	1.34	1.27

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:GLU:HB3	4:A:610:HOH:O	1.33	1.25
1:C:143:MET:SD	4:C:702:HOH:O	2.00	1.19
1:F:315:GLY:O	1:F:333:TYR:HB3	1.37	1.18
1:F:157:SER:C	4:F:601:HOH:O	1.82	1.18
1:A:90:ILE:CB	4:A:602:HOH:O	1.87	1.18
1:F:158:ASP:N	4:F:601:HOH:O	1.81	1.13
1:C:95:PRO:C	4:C:601:HOH:O	1.84	1.12
1:A:100[B]:ARG:NH1	4:A:601:HOH:O	1.82	1.12
1:D:391:VAL:N	4:D:602:HOH:O	1.83	1.11
1:C:364:ARG:NH1	4:C:603:HOH:O	1.82	1.09
1:A:182:VAL:N	4:A:603:HOH:O	1.85	1.07
1:A:315:GLY:O	1:A:333:TYR:HB3	1.52	1.07
1:C:433:ARG:NH2	4:C:607:HOH:O	1.88	1.06
1:B:249:LYS:HB2	4:B:607:HOH:O	1.59	1.03
1:A:41:GLU:N	4:A:604:HOH:O	1.91	1.02
1:B:432:GLN:CB	4:B:604:HOH:O	2.08	1.01
1:F:349:GLU:N	4:F:603:HOH:O	1.92	1.01
1:D:405:LYS:HD3	4:D:733:HOH:O	1.59	1.00
1:D:158:ASP:O	1:D:161:ASP:O	1.79	0.99
2:B:501:SF4:S1	4:B:678:HOH:O	2.20	0.98
1:F:435:ASN:OD1	4:F:602:HOH:O	1.82	0.98
1:B:250:ALA:N	4:B:607:HOH:O	1.97	0.97
1:A:433:ARG:NH2	4:A:605:HOH:O	1.96	0.97
1:C:94:GLU:O	4:C:601:HOH:O	1.80	0.97
1:C:321:LYS:O	4:C:602:HOH:O	1.81	0.97
1:B:254:GLU:OE1	4:B:601:HOH:O	1.84	0.95
1:A:90:ILE:CG1	4:A:602:HOH:O	2.10	0.95
1:E:266:ASP:OD2	4:E:601:HOH:O	1.82	0.95
1:A:90:ILE:HB	4:A:602:HOH:O	1.54	0.94
1:C:91:GLU:OE2	4:C:605:HOH:O	1.86	0.94
1:C:103:LYS:O	4:C:604:HOH:O	1.84	0.93
1:A:90:ILE:N	4:A:602:HOH:O	1.83	0.92
1:B:408:GLU:OE2	4:B:602:HOH:O	1.87	0.92
1:D:226:GLU:OE1	4:D:604:HOH:O	1.89	0.90
1:E:262:GLU:OE2	4:E:602:HOH:O	1.88	0.90
1:C:220:GLU:OE2	4:C:606:HOH:O	1.87	0.90
1:A:217:ARG:NH2	4:A:608:HOH:O	2.03	0.90
1:D:457:LYS:NZ	4:D:610:HOH:O	2.05	0.90
1:B:432:GLN:HB3	4:B:604:HOH:O	1.69	0.89
1:B:393:ASN:O	4:B:605:HOH:O	1.90	0.89
1:F:132:TRP:O	1:F:328:THR:HA	1.71	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:323:SER:O	1:E:368:THR:HG21	1.72	0.89
1:D:162:ARG:NH2	4:D:607:HOH:O	2.02	0.89
1:B:432:GLN:N	4:B:604:HOH:O	1.90	0.89
1:F:315:GLY:O	1:F:333:TYR:CB	2.20	0.89
1:E:60:ASP:HA	4:E:613:HOH:O	1.72	0.88
1:A:181:GLY:HA2	4:A:603:HOH:O	1.74	0.87
1:D:116:GLN:OE1	4:D:605:HOH:O	1.92	0.86
1:A:90:ILE:HG13	4:A:602:HOH:O	1.69	0.86
1:C:433:ARG:CZ	4:C:607:HOH:O	2.22	0.86
1:C:60:ASP:O	4:C:610:HOH:O	1.94	0.85
1:C:275:ASP:OD1	4:C:609:HOH:O	1.94	0.85
1:F:443:LYS:NZ	4:F:606:HOH:O	2.00	0.84
1:D:166:ARG:NH1	4:D:603:HOH:O	1.87	0.84
1:A:87:MET:O	4:A:602:HOH:O	1.96	0.83
1:B:339:GLU:OE1	4:B:606:HOH:O	1.96	0.82
1:A:220:GLU:O	4:A:606:HOH:O	1.96	0.82
1:F:166:ARG:HB2	4:F:601:HOH:O	1.81	0.81
1:A:315:GLY:O	1:A:333:TYR:CB	2.27	0.81
1:F:432:GLN:OE1	4:F:605:HOH:O	1.99	0.81
1:A:53:GLY:O	4:A:607:HOH:O	2.00	0.80
1:D:392:GLY:N	4:D:602:HOH:O	2.09	0.80
1:E:447:GLU:OE1	4:E:603:HOH:O	1.98	0.80
1:C:132:TRP:O	1:C:328:THR:HA	1.81	0.80
1:D:191:ASN:HB2	4:D:632:HOH:O	1.82	0.79
1:B:362:ASP:OD1	4:B:608:HOH:O	1.98	0.79
1:D:343:GLU:OE2	4:D:606:HOH:O	2.00	0.79
1:E:60:ASP:CA	4:E:613:HOH:O	2.28	0.79
1:C:364:ARG:CZ	4:C:603:HOH:O	2.20	0.78
1:C:95:PRO:CA	4:C:601:HOH:O	2.24	0.78
1:E:214:GLN:OE1	4:E:604:HOH:O	2.00	0.78
1:D:456:ASP:OD1	4:D:608:HOH:O	2.02	0.78
1:D:166:ARG:NH2	4:D:603:HOH:O	2.11	0.77
1:A:131:GLN:HB2	4:A:603:HOH:O	1.84	0.77
1:F:348:VAL:C	4:F:603:HOH:O	2.18	0.77
1:C:221:GLN:NE2	4:C:612:HOH:O	2.09	0.77
1:F:324:GLY:CA	4:F:612:HOH:O	2.33	0.77
1:A:158:ASP:O	1:A:161:ASP:O	2.02	0.76
1:E:64:GLN:NE2	4:E:608:HOH:O	2.10	0.76
1:F:166:ARG:CB	4:F:601:HOH:O	2.33	0.76
1:B:123:LYS:O	4:B:611:HOH:O	2.03	0.76
1:F:349:GLU:OE1	4:F:607:HOH:O	2.03	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:374:ASP:OD1	4:E:605:HOH:O	2.04	0.76
1:D:156:GLN:OE1	4:D:603:HOH:O	2.04	0.76
1:E:194:GLU:OE1	4:E:607:HOH:O	2.04	0.76
1:C:456:ASP:O	4:C:611:HOH:O	2.04	0.75
1:E:381:GLN:O	4:E:606:HOH:O	2.03	0.75
1:D:449:TYR:O	4:D:609:HOH:O	2.04	0.75
1:F:450:ASN:ND2	4:F:611:HOH:O	2.19	0.74
1:F:324:GLY:N	4:F:612:HOH:O	2.20	0.74
1:B:89:ARG:NH2	4:B:619:HOH:O	2.20	0.74
1:C:321:LYS:C	4:C:602:HOH:O	2.22	0.74
1:E:262:GLU:CD	4:E:602:HOH:O	2.24	0.73
1:D:94:GLU:OE1	4:D:611:HOH:O	2.05	0.73
1:E:416:TYR:OH	4:E:605:HOH:O	2.02	0.73
1:D:156:GLN:O	1:D:166:ARG:N	2.20	0.73
1:A:193:LEU:N	4:A:613:HOH:O	2.21	0.72
1:B:263:PHE:O	4:B:613:HOH:O	2.08	0.72
1:D:342:LYS:NZ	4:D:601:HOH:O	1.80	0.71
1:A:191:ASN:O	1:A:192:THR:OG1	2.07	0.70
1:E:132:TRP:O	1:E:328:THR:HA	1.91	0.70
1:A:191:ASN:C	4:A:613:HOH:O	2.30	0.69
1:B:411:ARG:NH2	4:B:610:HOH:O	2.03	0.69
1:A:264:MET:SD	4:A:678:HOH:O	2.50	0.69
1:F:451:LYS:O	4:F:609:HOH:O	2.09	0.69
1:D:171:ARG:CG	4:D:615:HOH:O	2.41	0.69
1:B:249:LYS:C	4:B:607:HOH:O	2.30	0.68
1:A:217:ARG:NH1	1:A:309:LEU:O	2.27	0.68
1:B:132:TRP:O	1:B:328:THR:HA	1.94	0.68
1:A:132:TRP:O	1:A:328:THR:HA	1.94	0.68
1:D:256:GLU:CG	4:D:613:HOH:O	2.41	0.68
1:B:433:ARG:NH2	4:B:617:HOH:O	2.17	0.68
1:B:103:LYS:O	4:B:615:HOH:O	2.12	0.67
1:A:112:PHE:O	1:A:337:ARG:NH2	2.26	0.67
1:C:182:VAL:HG13	3:C:503:FAD:HM82	1.76	0.67
1:E:122:ARG:NH1	1:E:353:GLU:OE2	2.28	0.67
1:D:84:GLY:O	1:D:433:ARG:NH2	2.28	0.67
1:D:112:PHE:O	1:D:337:ARG:NH2	2.28	0.66
1:A:117:GLU:OE1	4:A:610:HOH:O	2.14	0.66
1:E:261:TYR:O	4:E:609:HOH:O	2.12	0.66
1:D:291:LEU:O	1:D:294:VAL:HG22	1.95	0.66
1:C:158:ASP:O	1:C:161:ASP:O	2.14	0.65
1:A:315:GLY:O	1:A:333:TYR:N	2.29	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:339:GLU:CD	4:B:606:HOH:O	2.33	0.64
1:D:217:ARG:NH2	4:D:628:HOH:O	2.31	0.64
1:F:182:VAL:HG13	3:F:503:FAD:HM82	1.79	0.64
1:A:131:GLN:OE1	4:A:603:HOH:O	2.15	0.64
1:A:254:GLU:HA	1:E:256:GLU:HG3	1.80	0.64
1:D:256:GLU:OE2	4:D:613:HOH:O	2.15	0.64
1:B:249:LYS:CB	4:B:607:HOH:O	2.29	0.63
1:B:184:PRO:HG2	1:B:244:LEU:HD11	1.79	0.63
1:D:166:ARG:CZ	4:D:603:HOH:O	2.29	0.63
1:C:252:SER:HB2	1:C:271:LEU:HD22	1.80	0.63
1:D:390:PHE:C	4:D:602:HOH:O	2.23	0.63
1:B:159:PRO:HD3	1:B:166:ARG:HE	1.63	0.62
1:F:389:LEU:O	1:F:393:ASN:ND2	2.32	0.62
1:E:262:GLU:OE1	4:E:602:HOH:O	2.16	0.62
1:A:223:LEU:HB3	1:A:225:LEU:HD13	1.80	0.62
1:E:384:ALA:N	4:E:606:HOH:O	2.32	0.61
1:A:389:LEU:O	1:A:393:ASN:ND2	2.33	0.61
1:D:217:ARG:O	4:D:614:HOH:O	2.16	0.61
1:F:180:ARG:HH11	1:F:180:ARG:HG2	1.65	0.61
1:C:95:PRO:O	4:C:601:HOH:O	2.06	0.61
1:A:43:TRP:O	1:A:47:SER:OG	2.17	0.61
1:B:249:LYS:CA	4:B:607:HOH:O	2.47	0.61
3:D:503:FAD:H6	4:D:715:HOH:O	2.00	0.61
1:A:315:GLY:O	1:A:333:TYR:CA	2.48	0.61
1:D:43:TRP:O	1:D:47:SER:OG	2.18	0.60
1:F:80:CYS:O	1:F:89:ARG:NH2	2.29	0.60
1:D:122:ARG:HB3	1:D:331:PRO:HA	1.83	0.60
1:A:305:TYR:OH	4:A:611:HOH:O	2.15	0.60
1:B:112:PHE:O	1:B:337:ARG:NH2	2.34	0.60
1:F:184:PRO:HG2	1:F:244:LEU:HD11	1.82	0.60
1:D:202:LYS:HE3	1:D:226:GLU:HG3	1.83	0.59
1:A:448:MET:O	1:A:451:LYS:NZ	2.36	0.59
1:B:86:GLY:HA3	1:B:437:HIS:HD2	1.67	0.59
1:D:132:TRP:O	1:D:328:THR:HA	2.01	0.59
1:B:162:ARG:NH2	1:B:256:GLU:O	2.35	0.59
1:C:241:ARG:NH2	4:C:618:HOH:O	2.28	0.59
1:D:440:SER:OG	1:D:444:LYS:NZ	2.35	0.59
1:E:219:VAL:O	1:E:219:VAL:HG12	2.01	0.59
1:D:171:ARG:HG3	4:D:615:HOH:O	2.03	0.58
1:E:184:PRO:HG2	1:E:244:LEU:HD11	1.85	0.58
1:A:115:HIS:HA	1:A:337:ARG:HA	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:156:GLN:O	1:D:166:ARG:HB3	2.04	0.58
1:A:184:PRO:HG2	1:A:244:LEU:HD11	1.84	0.58
1:B:393:ASN:ND2	4:B:627:HOH:O	2.37	0.57
1:D:256:GLU:HG2	4:D:613:HOH:O	2.03	0.57
1:B:234:ASN:HD22	1:B:306:THR:HA	1.69	0.57
1:C:440:SER:OG	1:C:444:LYS:NZ	2.36	0.57
1:B:400:ASN:O	1:B:405:LYS:NZ	2.35	0.56
1:B:54:GLY:O	1:B:55:THR:HB	2.06	0.56
1:C:401:LEU:HD12	1:C:402:VAL:HG13	1.87	0.56
1:C:389:LEU:O	1:C:393:ASN:ND2	2.37	0.56
1:A:182:VAL:HG13	3:A:503:FAD:HM82	1.87	0.56
1:C:143:MET:HE1	1:C:344:MET:HG2	1.88	0.56
1:D:340:ARG:NH1	4:D:633:HOH:O	2.39	0.56
1:E:72:TYR:OH	1:E:197:GLU:OE2	2.19	0.56
1:E:394:ILE:HD12	1:F:395:ILE:HD13	1.88	0.56
1:E:182:VAL:HG13	3:E:503:FAD:HM82	1.87	0.56
1:E:319:VAL:HG23	1:E:333:TYR:HB2	1.88	0.56
1:B:115:HIS:HA	1:B:337:ARG:HA	1.89	0.55
1:A:202:LYS:HE3	1:A:226:GLU:HG3	1.88	0.55
1:B:129:GLY:HA3	1:B:180:ARG:HE	1.71	0.55
1:D:252:SER:HB2	1:D:271:LEU:HD22	1.89	0.55
1:B:389:LEU:O	1:B:391:VAL:N	2.36	0.55
1:B:450:ASN:O	1:B:450:ASN:ND2	2.39	0.55
1:E:194:GLU:HB2	4:E:632:HOH:O	2.06	0.54
1:C:304:ASP:OD2	4:C:615:HOH:O	2.18	0.54
1:A:313:VAL:HB	1:A:335:THR:HB	1.90	0.54
1:B:122:ARG:HG3	1:B:353:GLU:HB3	1.90	0.54
1:C:112:PHE:O	1:C:337:ARG:NH2	2.40	0.54
1:A:252:SER:HB2	1:A:271:LEU:HD22	1.89	0.54
1:B:158:ASP:O	4:B:618:HOH:O	2.19	0.54
1:B:335:THR:OG1	4:B:603:HOH:O	1.90	0.54
1:F:324:GLY:HA2	4:F:612:HOH:O	2.02	0.54
1:F:202:LYS:HE3	1:F:226:GLU:HG3	1.88	0.54
1:A:264:MET:HE2	1:A:270:GLN:HB3	1.90	0.53
1:C:148:MET:O	4:C:614:HOH:O	2.17	0.53
1:C:305:TYR:OH	4:C:613:HOH:O	2.17	0.53
1:C:99:GLY:N	4:C:601:HOH:O	2.30	0.53
1:E:129:GLY:HA3	1:E:180:ARG:HE	1.73	0.53
1:D:171:ARG:NH1	4:D:615:HOH:O	2.20	0.53
1:F:261:TYR:N	4:F:616:HOH:O	2.31	0.53
1:A:156:GLN:OE1	1:A:166:ARG:NH2	2.41	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:TYR:OH	1:B:363:ARG:NH1	2.42	0.53
1:A:324:GLY:O	1:B:454:GLN:NE2	2.41	0.53
1:C:122:ARG:NE	1:C:353:GLU:OE1	2.42	0.52
1:F:231:LEU:HB2	1:F:344:MET:HE1	1.91	0.52
1:F:166:ARG:HB3	4:F:601:HOH:O	2.04	0.52
1:A:141:ILE:HG23	1:A:173:PRO:HB3	1.91	0.52
1:D:182:VAL:HG13	3:D:503:FAD:HM82	1.92	0.52
1:D:217:ARG:NH1	1:D:309:LEU:O	2.42	0.52
1:E:214:GLN:HA	1:E:309:LEU:HD12	1.92	0.52
1:A:405:LYS:HD2	4:A:620:HOH:O	2.08	0.51
1:D:449:TYR:HB3	4:D:609:HOH:O	2.10	0.51
1:E:217:ARG:HG3	1:E:309:LEU:HB3	1.91	0.51
1:E:426:ASN:OD1	4:E:610:HOH:O	2.19	0.51
1:A:181:GLY:CA	4:A:603:HOH:O	2.38	0.51
1:F:347:LEU:HD12	4:F:661:HOH:O	2.11	0.51
1:A:129:GLY:HA3	1:A:180:ARG:HE	1.76	0.51
1:C:103:LYS:HE3	1:C:106:SER:HB2	1.93	0.51
1:B:141:ILE:HG23	1:B:173:PRO:HB3	1.93	0.51
1:F:315:GLY:O	1:F:333:TYR:CA	2.59	0.51
1:F:180:ARG:NH1	1:F:180:ARG:HG2	2.25	0.50
1:B:313:VAL:HG21	1:B:337:ARG:HH11	1.76	0.50
1:F:450:ASN:CG	4:F:611:HOH:O	2.49	0.50
1:E:122:ARG:HB3	1:E:331:PRO:HA	1.92	0.50
1:C:202:LYS:HE3	1:C:226:GLU:HG3	1.92	0.50
1:B:103:LYS:NZ	4:B:612:HOH:O	2.04	0.50
1:C:143:MET:CE	4:C:702:HOH:O	2.46	0.50
1:A:384:ALA:N	4:A:627:HOH:O	2.45	0.50
1:D:115:HIS:HA	1:D:337:ARG:HA	1.94	0.50
1:D:102:ARG:HB3	1:D:109:ASP:HB3	1.92	0.50
1:E:122:ARG:HB2	1:E:133:THR:HG21	1.93	0.50
1:C:95:PRO:HA	4:C:601:HOH:O	1.99	0.50
1:C:111:TYR:O	4:C:616:HOH:O	2.19	0.49
1:E:219:VAL:CG1	1:E:219:VAL:O	2.60	0.49
1:E:428:LYS:NZ	4:E:621:HOH:O	2.42	0.49
1:F:181:GLY:O	3:F:503:FAD:H8A	2.12	0.49
1:A:50:ILE:HD13	1:A:68:CYS:HB3	1.95	0.49
1:E:150:GLU:HG3	1:E:201:VAL:HG13	1.94	0.49
1:C:158:ASP:HB3	1:C:161:ASP:O	2.13	0.49
1:C:187:SER:O	1:C:212:GLN:NE2	2.46	0.49
1:D:129:GLY:HA3	1:D:180:ARG:HE	1.77	0.49
1:B:184:PRO:O	1:B:185:THR:HG23	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:424:TYR:CE2	4:F:608:HOH:O	2.55	0.49
1:D:390:PHE:N	4:D:602:HOH:O	2.46	0.49
1:C:268:LYS:HG2	1:C:282:PRO:HA	1.95	0.48
1:C:59:LYS:HB2	4:C:628:HOH:O	2.13	0.48
1:A:363:ARG:HB2	1:A:412:TYR:HB2	1.94	0.48
1:D:158:ASP:HB3	1:D:161:ASP:O	2.13	0.48
1:B:408:GLU:CD	4:B:602:HOH:O	2.46	0.48
1:E:451:LYS:HE3	4:E:640:HOH:O	2.13	0.48
1:B:374:ASP:OD1	1:B:416:TYR:OH	2.29	0.48
1:B:103:LYS:CE	4:B:612:HOH:O	2.57	0.48
1:C:162:ARG:HG3	1:C:163:LEU:HD13	1.95	0.48
1:F:196:ILE:HG23	1:F:201:VAL:HB	1.95	0.48
1:F:122:ARG:HG3	1:F:133:THR:HG21	1.96	0.47
1:E:190:LEU:HD11	1:E:216:LEU:HG	1.96	0.47
1:A:71:TYR:CE2	1:A:194:GLU:HG2	2.49	0.47
1:C:328:THR:OG1	4:C:617:HOH:O	2.20	0.47
1:F:115:HIS:HA	1:F:337:ARG:HA	1.95	0.47
1:B:333:TYR:OH	4:B:603:HOH:O	2.15	0.47
1:D:388:PRO:O	4:D:602:HOH:O	2.20	0.47
1:A:136:VAL:HG11	3:A:503:FAD:H4B	1.97	0.47
1:E:302:CYS:O	1:E:421:ASN:ND2	2.39	0.47
1:D:57:PRO:HG2	1:D:76:VAL:HG21	1.96	0.47
1:E:245:ASP:OD1	1:E:249:LYS:NZ	2.48	0.47
1:D:156:GLN:O	1:D:166:ARG:CA	2.62	0.47
1:F:214:GLN:HA	1:F:309:LEU:HD12	1.97	0.47
1:A:315:GLY:C	1:A:333:TYR:HB3	2.30	0.46
1:F:424:TYR:HE2	4:F:608:HOH:O	1.95	0.46
1:C:57:PRO:HG2	1:C:76:VAL:HG21	1.96	0.46
1:D:194:GLU:HB2	4:D:637:HOH:O	2.13	0.46
1:E:181:GLY:O	3:E:503:FAD:H8A	2.15	0.46
1:B:183:LYS:O	1:B:185:THR:N	2.48	0.46
1:B:122:ARG:HB3	1:B:331:PRO:HA	1.98	0.46
1:E:120:TYR:CD1	1:E:319:VAL:HG22	2.51	0.46
1:E:71:TYR:OH	1:E:197:GLU:OE1	2.21	0.46
1:F:149:VAL:HA	1:F:203:ARG:HB3	1.98	0.46
1:F:257:THR:HG23	1:F:273:HIS:ND1	2.30	0.46
1:C:153:VAL:HG23	1:C:204:LEU:HD11	1.98	0.46
1:F:262:GLU:HA	4:F:621:HOH:O	2.15	0.46
1:A:291:LEU:HD12	1:A:294:VAL:HG11	1.98	0.45
1:F:203:ARG:NE	4:F:624:HOH:O	2.49	0.45
1:E:132:TRP:O	1:E:328:THR:CA	2.62	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:259:LEU:O	1:E:260:HIS:CD2	2.69	0.45
1:B:122:ARG:NH2	4:B:632:HOH:O	2.48	0.45
1:B:190:LEU:HD11	1:B:216:LEU:HG	1.99	0.45
1:C:231:LEU:HB2	1:C:344:MET:HE1	1.98	0.45
1:E:171:ARG:NH1	4:E:630:HOH:O	2.49	0.45
1:A:193:LEU:HA	1:A:196:ILE:HD12	1.98	0.45
1:C:275:ASP:CG	4:C:609:HOH:O	2.49	0.45
1:C:119:LEU:HD13	1:C:354:ILE:HG23	1.99	0.45
1:E:216:LEU:O	1:E:220:GLU:N	2.50	0.45
1:E:60:ASP:CB	4:E:613:HOH:O	2.61	0.45
1:F:107:LEU:HA	1:F:110:THR:HG22	1.98	0.45
1:D:398:ILE:HD11	1:E:399:LEU:HD12	1.99	0.45
1:A:192:THR:O	1:A:196:ILE:HG13	2.17	0.45
1:B:171:ARG:HB2	4:B:640:HOH:O	2.16	0.45
1:C:214:GLN:HA	1:C:309:LEU:HD12	1.99	0.45
1:F:185:THR:HG22	1:F:244:LEU:HD12	1.97	0.45
1:E:234:ASN:HD22	1:E:315:GLY:HA3	1.82	0.45
1:F:289:ASN:HA	1:F:290:ASP:HA	1.70	0.45
1:F:454:GLN:OE1	1:F:454:GLN:N	2.48	0.45
1:A:117:GLU:CB	4:A:610:HOH:O	2.17	0.45
1:C:44:ARG:NH2	1:C:197:GLU:OE2	2.41	0.45
1:D:68:CYS:SG	1:D:73:ILE:HG13	2.57	0.45
1:E:115:HIS:HA	1:E:337:ARG:HA	1.99	0.45
1:B:54:GLY:O	1:B:55:THR:CB	2.65	0.45
1:C:422:TYR:O	1:C:426:ASN:ND2	2.34	0.45
1:C:340:ARG:O	1:C:344:MET:HG3	2.16	0.44
1:C:364:ARG:HD2	4:C:603:HOH:O	2.17	0.44
1:D:122:ARG:HB2	1:D:133:THR:HG21	1.98	0.44
1:B:174:GLU:N	1:B:174:GLU:OE1	2.49	0.44
1:E:112:PHE:O	1:E:337:ARG:NH2	2.50	0.44
1:B:217:ARG:HG3	1:B:309:LEU:HB3	1.99	0.44
1:D:102:ARG:NH2	4:D:612:HOH:O	2.09	0.44
1:D:323:SER:C	1:E:368:THR:HG21	2.36	0.44
1:A:122:ARG:NH2	1:A:353:GLU:OE1	2.49	0.44
1:D:259:LEU:O	1:D:260:HIS:CD2	2.70	0.44
1:E:371:VAL:HG12	1:E:416:TYR:HD1	1.82	0.44
1:A:260:HIS:O	1:A:272:LYS:N	2.46	0.44
1:C:313:VAL:HG21	1:C:337:ARG:HH11	1.82	0.44
1:E:377:ALA:HA	4:E:652:HOH:O	2.17	0.44
1:A:191:ASN:CA	4:A:613:HOH:O	2.66	0.44
1:E:68:CYS:SG	1:E:73:ILE:HG13	2.58	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:136:VAL:HG11	3:D:503:FAD:H4B	1.98	0.44
1:A:259:LEU:HD22	1:A:260:HIS:CE1	2.53	0.43
1:B:81:ALA:HB1	1:B:87:MET:HG2	2.00	0.43
1:D:187:SER:O	1:D:212:GLN:NE2	2.50	0.43
1:F:71:TYR:CE2	1:F:194:GLU:HG3	2.53	0.43
1:C:115:HIS:HA	1:C:337:ARG:HA	2.00	0.43
1:E:81:ALA:HB1	1:E:87:MET:HG2	1.99	0.43
1:F:217:ARG:HG3	1:F:309:LEU:HB3	2.00	0.43
1:F:427:ARG:NH2	1:F:458:MET:O	2.51	0.43
1:C:136:VAL:HG11	3:C:503:FAD:H4B	2.00	0.43
1:E:252:SER:HB2	1:E:271:LEU:HD22	1.99	0.43
1:E:452:ASN:OD1	4:E:611:HOH:O	2.21	0.43
1:F:158:ASP:CA	4:F:601:HOH:O	2.51	0.43
1:F:138:THR:HG22	1:F:348:VAL:HG11	2.00	0.43
1:D:444:LYS:O	1:D:448:MET:HG3	2.18	0.43
1:F:102:ARG:NE	1:F:113:GLY:HA2	2.34	0.43
1:F:202:LYS:NZ	1:F:224:ASN:O	2.43	0.43
1:C:181:GLY:O	3:C:503:FAD:H8A	2.19	0.43
1:F:144:LEU:HD23	1:F:149:VAL:HG23	2.00	0.43
1:A:234:ASN:HD22	1:A:306:THR:HA	1.84	0.43
1:E:121:ALA:HB3	1:E:334:ILE:HD12	1.99	0.43
1:F:133:THR:OG1	1:F:332:GLN:OE1	2.27	0.43
1:A:118:GLN:NE2	1:A:333:TYR:OH	2.50	0.43
1:D:425:VAL:O	1:D:429:TRP:HB2	2.19	0.43
1:A:181:GLY:O	3:A:503:FAD:H8A	2.18	0.43
1:C:158:ASP:OD1	1:C:160:GLU:HG2	2.19	0.43
3:C:503:FAD:H1'1	3:C:503:FAD:H9	1.85	0.43
1:A:71:TYR:OH	1:A:197:GLU:OE1	2.27	0.43
1:B:102:ARG:HB3	1:B:109:ASP:HB3	2.01	0.43
1:A:269:VAL:HB	1:A:281:VAL:HG13	2.01	0.42
1:D:234:ASN:HD22	1:D:306:THR:HA	1.84	0.42
1:D:313:VAL:HB	1:D:335:THR:HB	2.01	0.42
1:E:438:MET:HA	1:E:439:PRO:HD3	1.90	0.42
1:A:214:GLN:OE1	4:A:614:HOH:O	2.21	0.42
1:C:143:MET:HG2	1:C:148:MET:HE2	2.01	0.42
1:D:290:ASP:O	4:D:616:HOH:O	2.21	0.42
1:D:390:PHE:HE2	1:E:284:PHE:HB3	1.84	0.42
1:E:85:ASP:O	1:E:88:SER:OG	2.24	0.42
1:D:390:PHE:CE2	1:E:284:PHE:HB3	2.54	0.42
1:F:161:ASP:OD2	1:F:164:SER:OG	2.30	0.42
1:C:164:SER:HA	1:C:165:PRO:HD3	1.81	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:177:LEU:O	1:C:180:ARG:HD3	2.20	0.42
1:C:259:LEU:HG	1:C:274:LEU:HD23	2.01	0.42
1:C:259:LEU:HD22	1:C:260:HIS:CD2	2.55	0.42
1:E:287:PRO:HA	1:E:386:PRO:HG3	2.02	0.42
1:A:435:ASN:O	1:A:443:LYS:NZ	2.47	0.42
1:D:156:GLN:O	1:D:166:ARG:CB	2.66	0.42
1:D:346:SER:HA	1:D:349:GLU:HG3	2.02	0.42
1:B:315:GLY:O	1:B:333:TYR:N	2.49	0.42
1:F:122:ARG:HB2	1:F:331:PRO:HA	2.00	0.42
1:A:65:CYS:HB2	1:A:212:GLN:HG2	2.02	0.42
1:B:193:LEU:HA	1:B:196:ILE:HD12	2.01	0.42
3:E:503:FAD:H9	3:E:503:FAD:H1'1	1.88	0.42
1:F:259:LEU:O	1:F:260:HIS:CD2	2.73	0.42
1:B:214:GLN:HA	1:B:309:LEU:HD12	2.02	0.41
1:B:235:CYS:HA	3:B:503:FAD:N5	2.35	0.41
1:D:424:TYR:CE2	1:D:428:LYS:HD2	2.54	0.41
1:E:224:ASN:HB3	4:E:658:HOH:O	2.19	0.41
1:A:187:SER:O	1:A:212:GLN:NE2	2.54	0.41
1:B:251:ALA:O	1:B:281:VAL:HG21	2.20	0.41
1:B:86:GLY:HA3	1:B:437:HIS:CD2	2.50	0.41
1:E:91:GLU:OE2	1:E:440:SER:HB3	2.20	0.41
1:A:70:THR:HB	1:A:194:GLU:HG3	2.01	0.41
1:D:143:MET:HB3	1:D:149:VAL:HG22	2.02	0.41
3:F:503:FAD:H9	3:F:503:FAD:H1'1	1.85	0.41
1:B:150:GLU:HG3	1:B:203:ARG:HB2	2.02	0.41
1:C:160:GLU:HA	4:C:662:HOH:O	2.20	0.41
1:F:315:GLY:O	1:F:333:TYR:N	2.53	0.41
1:C:326:ASN:HB2	4:C:617:HOH:O	2.20	0.41
1:F:136:VAL:HG11	3:F:503:FAD:H4B	2.02	0.41
1:B:394:ILE:HD13	1:C:395:ILE:HD13	2.01	0.41
1:F:122:ARG:O	1:F:353:GLU:N	2.52	0.41
1:A:193:LEU:CG	4:A:613:HOH:O	2.21	0.41
1:A:319:VAL:HA	1:A:320:PRO:HD3	1.97	0.41
1:B:136:VAL:HG11	3:B:503:FAD:H4B	2.03	0.41
1:F:82:PHE:CZ	1:F:298:SER:HB2	2.56	0.41
1:B:184:PRO:O	1:B:244:LEU:HG	2.20	0.41
3:D:503:FAD:H9	3:D:503:FAD:H1'1	1.86	0.41
1:A:193:LEU:CB	4:A:613:HOH:O	2.64	0.41
1:B:366:PHE:CE1	1:B:399:LEU:HD12	2.55	0.41
1:D:281:VAL:HA	1:D:282:PRO:HD3	1.90	0.41
1:D:358:ILE:O	1:D:406:GLY:HA3	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:394:ILE:H	1:E:394:ILE:HG12	1.59	0.41
1:A:366:PHE:HE1	1:A:399:LEU:HG	1.84	0.41
1:B:301:SER:O	1:B:437:HIS:HE1	2.04	0.41
1:C:59:LYS:CB	4:C:628:HOH:O	2.68	0.41
1:F:239:GLY:HA2	1:F:296:ALA:HB2	2.03	0.41
1:A:385:GLN:HA	1:A:386:PRO:HD3	1.85	0.40
1:B:132:TRP:CZ3	1:B:330:HIS:HB3	2.56	0.40
1:F:68:CYS:SG	1:F:73:ILE:HG13	2.61	0.40
1:A:452:ASN:HB2	1:A:454:GLN:NE2	2.36	0.40
1:B:65:CYS:HB2	1:B:212:GLN:HG2	2.03	0.40
1:E:317:MET:HB3	4:E:612:HOH:O	2.21	0.40
1:B:53:GLY:HA2	1:B:54:GLY:HA3	1.61	0.40
1:C:190:LEU:HG	1:C:193:LEU:HD11	2.04	0.40
1:D:359:SER:HB2	1:D:407:LEU:HB2	2.04	0.40
1:E:341:GLY:HA2	1:E:344:MET:HE3	2.03	0.40
1:B:82:PHE:CZ	1:B:298:SER:HB2	2.57	0.40
1:C:221:GLN:HB2	4:C:612:HOH:O	2.21	0.40
1:D:153:VAL:HG23	1:D:204:LEU:HD11	2.04	0.40
1:C:319:VAL:HA	1:C:320:PRO:HD3	1.95	0.40
1:D:322:TYR:CE1	1:D:331:PRO:HG2	2.56	0.40

All (7) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:GLY:O	1:C:350:ASN:CB[1_565]	1.68	0.52
4:D:622:HOH:O	4:E:705:HOH:O[3_555]	1.87	0.33
4:A:681:HOH:O	4:D:749:HOH:O[1_655]	1.95	0.25
4:A:621:HOH:O	4:E:666:HOH:O[1_655]	2.00	0.20
4:D:720:HOH:O	4:E:700:HOH:O[3_555]	2.03	0.17
4:C:689:HOH:O	4:E:689:HOH:O[3_545]	2.13	0.07
4:C:689:HOH:O	4:E:619:HOH:O[3_545]	2.16	0.04

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	411/437 (94%)	391 (95%)	17 (4%)	3 (1%)	26	55
1	B	410/437 (94%)	394 (96%)	14 (3%)	2 (0%)	34	63
1	C	420/437 (96%)	403 (96%)	17 (4%)	0	100	100
1	D	407/437 (93%)	393 (97%)	13 (3%)	1 (0%)	52	80
1	E	402/437 (92%)	387 (96%)	15 (4%)	0	100	100
1	F	412/437 (94%)	392 (95%)	19 (5%)	1 (0%)	52	80
All	All	2462/2622 (94%)	2360 (96%)	95 (4%)	7 (0%)	46	75

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	53	GLY
1	B	385	GLN
1	A	48	ARG
1	A	385	GLN
1	B	55	THR
1	D	48	ARG
1	A	54	GLY

5.3.2 Protein sidechains (i)

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	348/378 (92%)	337 (97%)	11 (3%)	46	77
1	B	345/378 (91%)	336 (97%)	9 (3%)	54	83
1	C	358/378 (95%)	344 (96%)	14 (4%)	39	70
1	D	345/378 (91%)	332 (96%)	13 (4%)	40	71
1	E	338/378 (89%)	329 (97%)	9 (3%)	52	82
1	F	349/378 (92%)	338 (97%)	11 (3%)	46	77
All	All	2083/2268 (92%)	2016 (97%)	67 (3%)	46	77

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	TYR
1	A	89	ARG
1	A	217	ARG
1	A	244	LEU
1	A	259	LEU
1	A	291	LEU
1	A	305	TYR
1	A	312	LEU
1	A	337	ARG
1	A	432	GLN
1	A	457	LYS
1	B	171	ARG
1	B	190	LEU
1	B	216	LEU
1	B	228	LEU
1	B	244	LEU
1	B	259	LEU
1	B	305	TYR
1	B	319	VAL
1	B	363	ARG
1	C	71	TYR
1	C	83	LEU
1	C	180	ARG
1	C	183	LYS
1	C	185	THR
1	C	209	VAL
1	C	241	ARG
1	C	244	LEU
1	C	259	LEU
1	C	305	TYR
1	C	317	MET
1	C	347	LEU
1	C	348	VAL
1	C	358	ILE
1	D	83	LEU
1	D	171	ARG
1	D	190	LEU
1	D	217	ARG
1	D	253	LYS
1	D	259	LEU
1	D	312	LEU
1	D	340	ARG

Continued on next page...

Full wwPDB X-ray Structure Validation Report

Continued from previous page...

Mol	Chain	Res	Type
1	D	358	ILE
1	D	364	ARG
1	D	389	LEU
1	D	433	ARG
1	D	438	MET
1	E	185	THR
1	E	216	LEU
1	E	228	LEU
1	E	244	LEU
1	E	256	GLU
1	E	259	LEU
1	E	312	LEU
1	E	317	MET
1	E	394	ILE
1	F	128	GLU
1	F	185	THR
1	F	205	LEU
1	F	209	VAL
1	F	244	LEU
1	F	259	LEU
1	F	305	TYR
1	F	312	LEU
1	F	348	VAL
1	F	397	PHE
1	F	432	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	118	GLN
1	A	260	HIS
1	B	437	HIS
1	D	116	GLN
1	E	260	HIS
1	F	432	GLN
1	F	435	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no 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	FAD	A	503	-	52,58,58	2.50	18 (34%)	52,89,89	2.30	10 (19%)
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	FAD	B	503	-	52,58,58	2.49	18 (34%)	52,89,89	2.27	10 (19%)
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	FAD	C	503	-	52,58,58	2.49	17 (32%)	52,89,89	2.27	10 (19%)
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	FAD	D	503	-	52,58,58	2.49	18 (34%)	52,89,89	2.32	10 (19%)
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	FAD	E	503	-	52,58,58	2.49	18 (34%)	52,89,89	2.28	8 (15%)
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	FAD	F	503	-	52,58,58	2.49	18 (34%)	52,89,89	2.31	10 (19%)

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	FAD	A	503	-	-	0/30/50/50	0/6/6/6
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	FAD	B	503	-	-	0/30/50/50	0/6/6/6
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	FAD	C	503	-	-	0/30/50/50	0/6/6/6
2	SF4	D	501	1	-	0/0/48/48	0/6/5/5
2	SF4	D	502	1	-	0/0/48/48	0/6/5/5
3	FAD	D	503	-	-	0/30/50/50	0/6/6/6
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	FAD	E	503	-	-	0/30/50/50	0/6/6/6
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	FAD	F	503	-	-	0/30/50/50	0/6/6/6

All (107) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	503	FAD	C2B-C1B	-5.46	1.45	1.53
3	D	503	FAD	C2B-C1B	-5.45	1.45	1.53
3	A	503	FAD	C2B-C1B	-5.44	1.45	1.53
3	F	503	FAD	C2B-C1B	-5.40	1.45	1.53
3	B	503	FAD	C2B-C1B	-5.37	1.45	1.53
3	C	503	FAD	C2B-C1B	-5.35	1.45	1.53
3	E	503	FAD	C2B-C3B	-3.96	1.42	1.53
3	D	503	FAD	C2B-C3B	-3.94	1.42	1.53
3	A	503	FAD	C2B-C3B	-3.93	1.42	1.53
3	C	503	FAD	C2B-C3B	-3.90	1.42	1.53
3	F	503	FAD	C2B-C3B	-3.88	1.43	1.53
3	B	503	FAD	C2B-C3B	-3.82	1.43	1.53
3	D	503	FAD	C3B-C4B	-2.69	1.45	1.53
3	C	503	FAD	C3B-C4B	-2.66	1.45	1.53
3	B	503	FAD	O3'-C3'	-2.64	1.36	1.43
3	F	503	FAD	C3B-C4B	-2.64	1.45	1.53
3	E	503	FAD	C3B-C4B	-2.62	1.46	1.53
3	A	503	FAD	C3B-C4B	-2.62	1.46	1.53
3	D	503	FAD	O3'-C3'	-2.61	1.36	1.43

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	503	FAD	C3B-C4B	-2.60	1.46	1.53
3	A	503	FAD	O3'-C3'	-2.57	1.36	1.43
3	F	503	FAD	O3'-C3'	-2.56	1.36	1.43
3	C	503	FAD	O3'-C3'	-2.55	1.37	1.43
3	E	503	FAD	O3'-C3'	-2.54	1.37	1.43
3	E	503	FAD	O4'-C4'	-2.49	1.37	1.43
3	B	503	FAD	O4'-C4'	-2.48	1.37	1.43
3	A	503	FAD	O4'-C4'	-2.45	1.37	1.43
3	D	503	FAD	O4'-C4'	-2.44	1.37	1.43
3	C	503	FAD	O4'-C4'	-2.40	1.38	1.43
3	F	503	FAD	O4'-C4'	-2.38	1.38	1.43
3	D	503	FAD	C4'-C3'	-2.22	1.49	1.53
3	D	503	FAD	O2'-C2'	-2.20	1.38	1.43
3	F	503	FAD	O2'-C2'	-2.19	1.38	1.43
3	B	503	FAD	O2'-C2'	-2.18	1.38	1.43
3	C	503	FAD	O2'-C2'	-2.16	1.38	1.43
3	E	503	FAD	O2'-C2'	-2.14	1.38	1.43
3	A	503	FAD	O2'-C2'	-2.13	1.38	1.43
3	E	503	FAD	C4'-C3'	-2.12	1.49	1.53
3	F	503	FAD	C4'-C3'	-2.06	1.49	1.53
3	B	503	FAD	C4'-C3'	-2.06	1.49	1.53
3	A	503	FAD	C4'-C3'	-2.03	1.49	1.53
3	F	503	FAD	C2-N3	2.39	1.43	1.38
3	C	503	FAD	C2-N3	2.40	1.43	1.38
3	B	503	FAD	C2-N3	2.40	1.43	1.38
3	E	503	FAD	C2-N3	2.43	1.43	1.38
3	A	503	FAD	C2-N3	2.44	1.43	1.38
3	D	503	FAD	C2-N3	2.50	1.43	1.38
3	A	503	FAD	C6A-N6A	2.63	1.44	1.34
3	F	503	FAD	C6A-N6A	2.64	1.45	1.34
3	E	503	FAD	C6A-N6A	2.65	1.45	1.34
3	D	503	FAD	C10-N10	2.66	1.42	1.39
3	C	503	FAD	C6A-N6A	2.67	1.45	1.34
3	B	503	FAD	C6A-N6A	2.67	1.45	1.34
3	D	503	FAD	C6A-N6A	2.69	1.45	1.34
3	E	503	FAD	C4-C4X	2.78	1.46	1.41
3	D	503	FAD	C2A-N3A	2.80	1.37	1.32
3	B	503	FAD	C4-C4X	2.82	1.47	1.41
3	D	503	FAD	C4-C4X	2.84	1.47	1.41
3	E	503	FAD	C2A-N3A	2.84	1.37	1.32
3	A	503	FAD	C2A-N3A	2.86	1.37	1.32
3	F	503	FAD	C2A-N3A	2.88	1.37	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	503	FAD	C2A-N3A	2.89	1.37	1.32
3	F	503	FAD	C4-C4X	2.90	1.47	1.41
3	C	503	FAD	C2A-N3A	2.91	1.37	1.32
3	C	503	FAD	C4-C4X	2.93	1.47	1.41
3	A	503	FAD	C4-C4X	2.96	1.47	1.41
3	F	503	FAD	C10-N10	2.98	1.42	1.39
3	E	503	FAD	C10-N10	3.05	1.42	1.39
3	C	503	FAD	C10-N10	3.11	1.42	1.39
3	A	503	FAD	C10-N10	3.12	1.42	1.39
3	B	503	FAD	C10-N10	3.13	1.42	1.39
3	D	503	FAD	C9A-N10	3.34	1.43	1.38
3	F	503	FAD	C9A-N10	3.34	1.43	1.38
3	C	503	FAD	C9A-N10	3.42	1.43	1.38
3	A	503	FAD	C9A-N10	3.46	1.43	1.38
3	B	503	FAD	C9A-N10	3.46	1.43	1.38
3	E	503	FAD	C9A-N10	3.54	1.43	1.38
3	F	503	FAD	O4B-C1B	3.68	1.46	1.41
3	A	503	FAD	O4B-C1B	3.75	1.46	1.41
3	C	503	FAD	O4B-C1B	3.75	1.46	1.41
3	D	503	FAD	O4B-C1B	3.78	1.46	1.41
3	B	503	FAD	O4B-C1B	3.87	1.46	1.41
3	E	503	FAD	O4B-C1B	3.87	1.46	1.41
3	F	503	FAD	C4-N3	4.03	1.40	1.33
3	C	503	FAD	C4-N3	4.03	1.40	1.33
3	B	503	FAD	C4-N3	4.03	1.40	1.33
3	E	503	FAD	C4-N3	4.05	1.40	1.33
3	D	503	FAD	C4-N3	4.06	1.40	1.33
3	A	503	FAD	C4-N3	4.08	1.40	1.33
3	D	503	FAD	C2-N1	4.49	1.47	1.38
3	C	503	FAD	C2-N1	4.57	1.47	1.38
3	A	503	FAD	C2-N1	4.58	1.47	1.38
3	B	503	FAD	C2-N1	4.60	1.47	1.38
3	E	503	FAD	C2-N1	4.60	1.47	1.38
3	F	503	FAD	C2-N1	4.61	1.47	1.38
3	F	503	FAD	C4X-C10	5.52	1.51	1.40
3	C	503	FAD	C4X-C10	5.57	1.51	1.40
3	E	503	FAD	C4X-C10	5.57	1.51	1.40
3	D	503	FAD	C4X-C10	5.58	1.51	1.40
3	B	503	FAD	C4X-C10	5.61	1.51	1.40
3	A	503	FAD	C4X-C10	5.63	1.51	1.40
3	E	503	FAD	C5X-N5	9.59	1.50	1.35
3	A	503	FAD	C5X-N5	9.66	1.50	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	503	FAD	C5X-N5	9.69	1.50	1.35
3	C	503	FAD	C5X-N5	9.69	1.50	1.35
3	D	503	FAD	C5X-N5	9.75	1.50	1.35
3	F	503	FAD	C5X-N5	9.80	1.50	1.35

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	503	FAD	N3A-C2A-N1A	-11.21	120.07	128.87
3	B	503	FAD	N3A-C2A-N1A	-11.04	120.19	128.87
3	A	503	FAD	N3A-C2A-N1A	-11.02	120.21	128.87
3	F	503	FAD	N3A-C2A-N1A	-11.00	120.23	128.87
3	E	503	FAD	N3A-C2A-N1A	-10.99	120.24	128.87
3	C	503	FAD	N3A-C2A-N1A	-10.83	120.37	128.87
3	E	503	FAD	C4X-C10-N10	-4.69	117.11	120.52
3	F	503	FAD	C4X-C10-N10	-4.64	117.15	120.52
3	A	503	FAD	C4X-C10-N10	-4.60	117.17	120.52
3	D	503	FAD	C4X-C10-N10	-4.56	117.20	120.52
3	C	503	FAD	C4X-C10-N10	-4.54	117.22	120.52
3	B	503	FAD	C4X-C10-N10	-4.39	117.33	120.52
3	F	503	FAD	C4B-O4B-C1B	-4.37	105.01	109.64
3	A	503	FAD	C4B-O4B-C1B	-4.33	105.06	109.64
3	F	503	FAD	N3-C2-N1	-4.30	120.44	127.69
3	D	503	FAD	N3-C2-N1	-4.26	120.52	127.69
3	E	503	FAD	C4B-O4B-C1B	-4.25	105.13	109.64
3	C	503	FAD	N3-C2-N1	-4.25	120.54	127.69
3	B	503	FAD	N3-C2-N1	-4.18	120.66	127.69
3	E	503	FAD	N3-C2-N1	-4.17	120.67	127.69
3	A	503	FAD	N3-C2-N1	-4.15	120.70	127.69
3	D	503	FAD	C4B-O4B-C1B	-4.14	105.25	109.64
3	C	503	FAD	C4B-O4B-C1B	-3.96	105.45	109.64
3	B	503	FAD	C4B-O4B-C1B	-3.92	105.48	109.64
3	F	503	FAD	C4-C4X-C10	-3.22	117.88	119.94
3	D	503	FAD	C4-C4X-C10	-3.12	117.95	119.94
3	C	503	FAD	C4-C4X-C10	-2.98	118.03	119.94
3	E	503	FAD	C4X-C4-N3	-2.81	119.84	123.52
3	D	503	FAD	C4X-C4-N3	-2.77	119.90	123.52
3	A	503	FAD	C4X-C4-N3	-2.77	119.91	123.52
3	B	503	FAD	C4X-C4-N3	-2.76	119.91	123.52
3	A	503	FAD	C4-C4X-C10	-2.71	118.20	119.94
3	C	503	FAD	C4X-C4-N3	-2.59	120.14	123.52
3	B	503	FAD	C4-C4X-C10	-2.58	118.29	119.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	503	FAD	C4-C4X-C10	-2.50	118.34	119.94
3	F	503	FAD	C4X-C4-N3	-2.47	120.30	123.52
3	D	503	FAD	C2B-C3B-C4B	2.04	106.80	102.64
3	B	503	FAD	C4-C4X-N5	2.07	121.21	118.70
3	A	503	FAD	C2B-C3B-C4B	2.14	107.02	102.64
3	B	503	FAD	C2B-C3B-C4B	2.29	107.33	102.64
3	A	503	FAD	C4-C4X-N5	2.31	121.51	118.70
3	C	503	FAD	C4-C4X-N5	2.33	121.53	118.70
3	F	503	FAD	C2B-C3B-C4B	2.33	107.40	102.64
3	C	503	FAD	C2B-C3B-C4B	2.40	107.54	102.64
3	F	503	FAD	C4-C4X-N5	2.44	121.67	118.70
3	D	503	FAD	C4-C4X-N5	2.45	121.68	118.70
3	B	503	FAD	C4X-N5-C5X	3.05	120.32	116.72
3	D	503	FAD	C4X-N5-C5X	3.13	120.42	116.72
3	E	503	FAD	C4X-N5-C5X	3.17	120.46	116.72
3	C	503	FAD	C4X-N5-C5X	3.19	120.48	116.72
3	F	503	FAD	C4X-N5-C5X	3.20	120.50	116.72
3	A	503	FAD	C4X-N5-C5X	3.27	120.58	116.72
3	F	503	FAD	C4-N3-C2	6.44	120.53	115.16
3	C	503	FAD	C4-N3-C2	6.45	120.54	115.16
3	A	503	FAD	C4-N3-C2	6.52	120.60	115.16
3	B	503	FAD	C4-N3-C2	6.52	120.60	115.16
3	E	503	FAD	C4-N3-C2	6.59	120.66	115.16
3	D	503	FAD	C4-N3-C2	6.73	120.77	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	503	FAD	3	0
2	B	501	SF4	1	0
3	B	503	FAD	2	0
3	C	503	FAD	4	0
3	D	503	FAD	4	0
3	E	503	FAD	3	0
3	F	503	FAD	4	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 (i)

6.1 Protein, DNA and RNA chains (i)

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(Å²)	Q<0.9
1	A	414/437 (94%)	0.26	23 (5%)	28	26	8, 18, 37, 68	24 (5%)
1	B	411/437 (94%)	0.03	7 (1%)	73	74	3, 11, 34, 53	21 (5%)
1	C	421/437 (96%)	0.07	5 (1%)	81	81	5, 15, 35, 53	16 (3%)
1	D	411/437 (94%)	-0.06	3 (0%)	89	90	1, 7, 29, 44	20 (4%)
1	E	406/437 (92%)	-0.01	2 (0%)	91	93	3, 13, 38, 56	12 (2%)
1	F	413/437 (94%)	0.39	24 (5%)	26	25	12, 26, 44, 59	13 (3%)
All	All	2476/2622 (94%)	0.11	64 (2%)	59	59	1, 15, 39, 68	106 (4%)

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	52	PRO	8.2
1	A	54	GLY	5.4
1	B	291	LEU	4.4
1	A	193	LEU	4.1
1	A	83	LEU	4.0
1	A	53	GLY	3.8
1	D	52	PRO	3.8
1	A	198	ALA	3.7
1	F	83	LEU	3.6
1	A	49	PRO	3.5
1	A	51	PRO	3.3
1	A	376	ALA	3.3
1	A	48	ARG	3.3
1	F	315	GLY	3.2
1	F	218	SER	3.1
1	A	56	TYR	3.0
1	F	93	LEU	3.0
1	A	72	TYR	2.9
1	C	303	PHE	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	371	VAL	2.9
1	C	425	VAL	2.9
1	C	429	TRP	2.8
1	E	378	LYS	2.8
1	C	432	GLN	2.7
1	F	92	SER	2.7
1	F	306	THR	2.7
1	F	390	PHE	2.6
1	F	102	ARG	2.6
1	A	55	THR	2.5
1	A	305	TYR	2.5
1	F	82	PHE	2.5
1	F	425	VAL	2.5
1	F	87	MET	2.5
1	A	190	LEU	2.4
1	F	90	ILE	2.4
1	B	381	GLN	2.4
1	A	50	ILE	2.4
1	B	54	GLY	2.4
1	F	206	PHE	2.4
1	F	88	SER	2.3
1	B	324	GLY	2.3
1	A	192	THR	2.3
1	A	429	TRP	2.3
1	A	47	SER	2.3
1	A	65	CYS	2.3
1	F	232	GLY	2.2
1	F	79	ALA	2.2
1	F	86	GLY	2.2
1	F	438	MET	2.2
1	F	214	GLN	2.1
1	A	364	ARG	2.1
1	D	46	LYS	2.1
1	F	389	LEU	2.1
1	A	64	GLN	2.1
1	B	177	LEU	2.1
1	C	437	HIS	2.1
1	F	260	HIS	2.1
1	F	350	ASN	2.0
1	F	309	LEU	2.0
1	B	378	LYS	2.0
1	D	53	GLY	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	84	GLY	2.0
1	E	83	LEU	2.0
1	B	383	PRO	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($Å^2$)	Q<0.9
3	FAD	B	503	53/53	0.94	0.19	0.32	3,5,9,11	0
3	FAD	D	503	53/53	0.95	0.18	0.29	1,1,2,3	0
3	FAD	C	503	53/53	0.95	0.18	0.11	3,6,9,10	0
3	FAD	E	503	53/53	0.96	0.17	-0.04	1,4,6,12	0
3	FAD	A	503	53/53	0.94	0.18	-0.24	6,11,13,15	0
2	SF4	B	501	8/8	0.96	0.14	-0.32	4,12,14,20	0
3	FAD	F	503	53/53	0.95	0.17	-0.56	8,12,17,20	0
2	SF4	B	502	8/8	0.93	0.14	-0.67	1,2,7,8	0
2	SF4	E	501	8/8	0.94	0.13	-0.70	8,12,18,23	0
2	SF4	F	501	8/8	0.95	0.12	-1.00	20,22,34,35	0
2	SF4	D	501	8/8	0.89	0.14	-1.14	2,9,13,13	0
2	SF4	C	501	8/8	0.92	0.13	-1.35	4,9,10,12	0
2	SF4	D	502	8/8	0.96	0.11	-1.37	1,2,4,5	0
2	SF4	A	502	8/8	0.93	0.10	-1.47	5,12,18,19	0
2	SF4	F	502	8/8	0.93	0.11	-1.97	6,13,21,23	0
2	SF4	E	502	8/8	0.94	0.11	-2.36	4,6,9,10	0
2	SF4	C	502	8/8	0.94	0.10	-2.41	3,5,10,15	0
2	SF4	A	501	8/8	0.97	0.07	-3.42	13,19,24,28	0

6.5 Other polymers (i)

There are no such residues in this entry.