



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2026 – 11:53 AM UTC

PDB ID : 2O78 / pdb_00002o78
Title : Tyrosine ammonia-lyase from *Rhodobacter sphaeroides* (His89Phe variant) complexed with cinnamic acid
Authors : Louie, G.V.; Bowman, M.E.; Moffitt, M.C.; Baiga, T.J.; Moore, B.S.; Noel, J.P.
Deposited on : 2006-12-10
Resolution : 1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

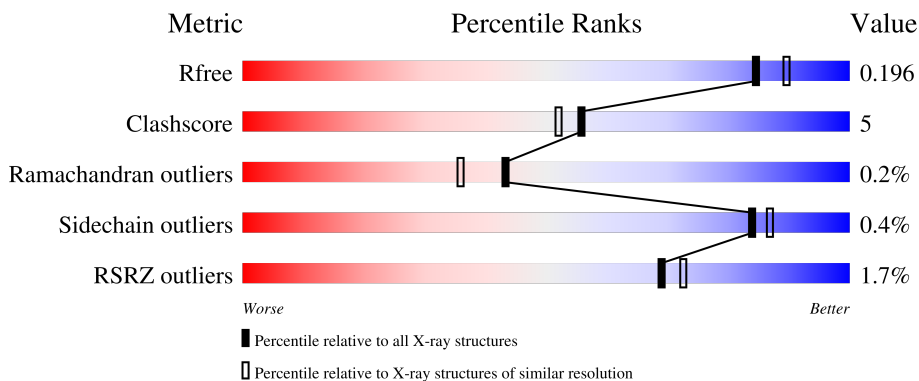
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	521	 3% 88% 10% ..
1	B	521	 2% 87% 11% ..
1	C	521	 % 87% 11% ..
1	D	521	 2% 85% 13% ..
1	E	521	 2% 89% 9% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	521	 89% 9% ..
1	G	521	 88% 9% ..
1	H	521	 3% 85% 12% ..

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 33846 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 Putative histidine ammonia-lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	515	3814	2366	729	705	14	0	0	0
1	B	515	3814	2366	729	705	14	0	0	0
1	C	514	3807	2361	728	704	14	0	0	0
1	D	514	3807	2361	728	704	14	0	0	0
1	E	514	3807	2361	728	704	14	0	0	0
1	F	514	3807	2361	728	704	14	0	0	0
1	G	514	3807	2361	728	704	14	0	0	0
1	H	514	3807	2361	728	704	14	0	0	0

There are 32 discrepancies between the modelled and reference sequences:

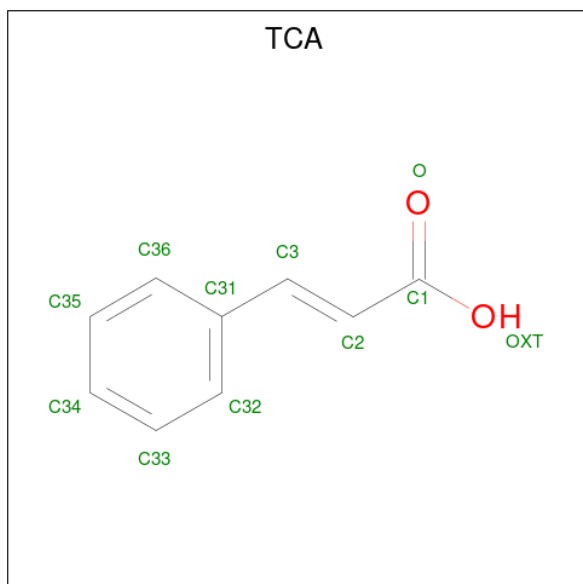
Chain	Residue	Modelled	Actual	Comment	Reference
A	89	PHE	HIS	engineered mutation	UNP Q3IWB0
A	149	MDO	ALA	SEE REMARK 999	UNP Q3IWB0
A	149	MDO	SER	SEE REMARK 999	UNP Q3IWB0
A	149	MDO	GLY	SEE REMARK 999	UNP Q3IWB0
B	89	PHE	HIS	engineered mutation	UNP Q3IWB0
B	149	MDO	ALA	SEE REMARK 999	UNP Q3IWB0
B	149	MDO	SER	SEE REMARK 999	UNP Q3IWB0
B	149	MDO	GLY	SEE REMARK 999	UNP Q3IWB0
C	89	PHE	HIS	engineered mutation	UNP Q3IWB0
C	149	MDO	ALA	SEE REMARK 999	UNP Q3IWB0
C	149	MDO	SER	SEE REMARK 999	UNP Q3IWB0
C	149	MDO	GLY	SEE REMARK 999	UNP Q3IWB0
D	89	PHE	HIS	engineered mutation	UNP Q3IWB0

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	149	MDO	ALA	SEE REMARK 999	UNP Q3IWB0
D	149	MDO	SER	SEE REMARK 999	UNP Q3IWB0
D	149	MDO	GLY	SEE REMARK 999	UNP Q3IWB0
E	89	PHE	HIS	engineered mutation	UNP Q3IWB0
E	149	MDO	ALA	SEE REMARK 999	UNP Q3IWB0
E	149	MDO	SER	SEE REMARK 999	UNP Q3IWB0
E	149	MDO	GLY	SEE REMARK 999	UNP Q3IWB0
F	89	PHE	HIS	engineered mutation	UNP Q3IWB0
F	149	MDO	ALA	SEE REMARK 999	UNP Q3IWB0
F	149	MDO	SER	SEE REMARK 999	UNP Q3IWB0
F	149	MDO	GLY	SEE REMARK 999	UNP Q3IWB0
G	89	PHE	HIS	engineered mutation	UNP Q3IWB0
G	149	MDO	ALA	SEE REMARK 999	UNP Q3IWB0
G	149	MDO	SER	SEE REMARK 999	UNP Q3IWB0
G	149	MDO	GLY	SEE REMARK 999	UNP Q3IWB0
H	89	PHE	HIS	engineered mutation	UNP Q3IWB0
H	149	MDO	ALA	SEE REMARK 999	UNP Q3IWB0
H	149	MDO	SER	SEE REMARK 999	UNP Q3IWB0
H	149	MDO	GLY	SEE REMARK 999	UNP Q3IWB0

- Molecule 2 is PHENYLETHYLENECARBOXYLIC ACID (CCD ID: TCA) (formula: C₉H₈O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			11	9	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C O 11 9 2	0	0
2	C	1	Total C O 11 9 2	0	0
2	D	1	Total C O 11 9 2	0	0
2	E	1	Total C O 11 9 2	0	0
2	F	1	Total C O 11 9 2	0	0
2	G	1	Total C O 11 9 2	0	0
2	H	1	Total C O 11 9 2	0	0

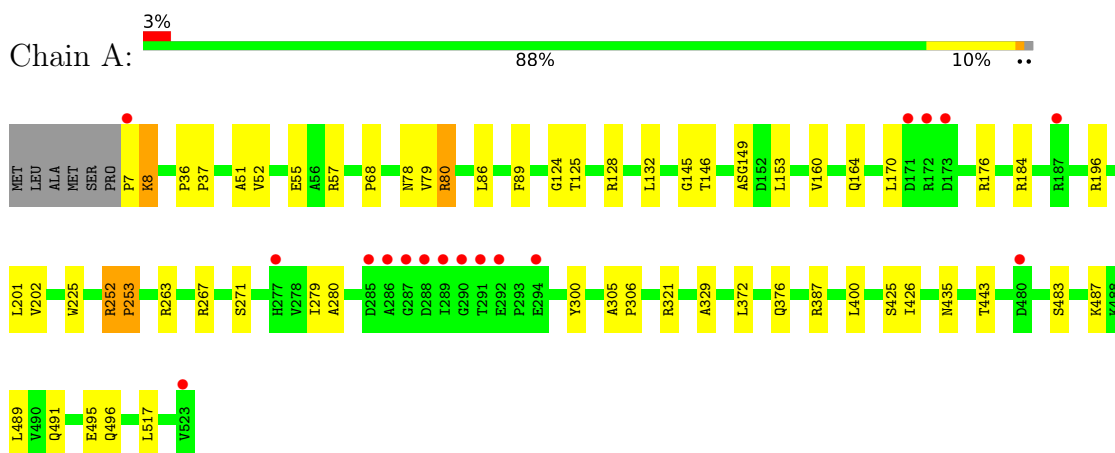
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	374	Total O 374 374	0	0
3	B	394	Total O 394 394	0	0
3	C	415	Total O 415 415	0	0
3	D	400	Total O 400 400	0	0
3	E	392	Total O 392 392	0	0
3	F	486	Total O 486 486	0	0
3	G	435	Total O 435 435	0	0
3	H	392	Total O 392 392	0	0

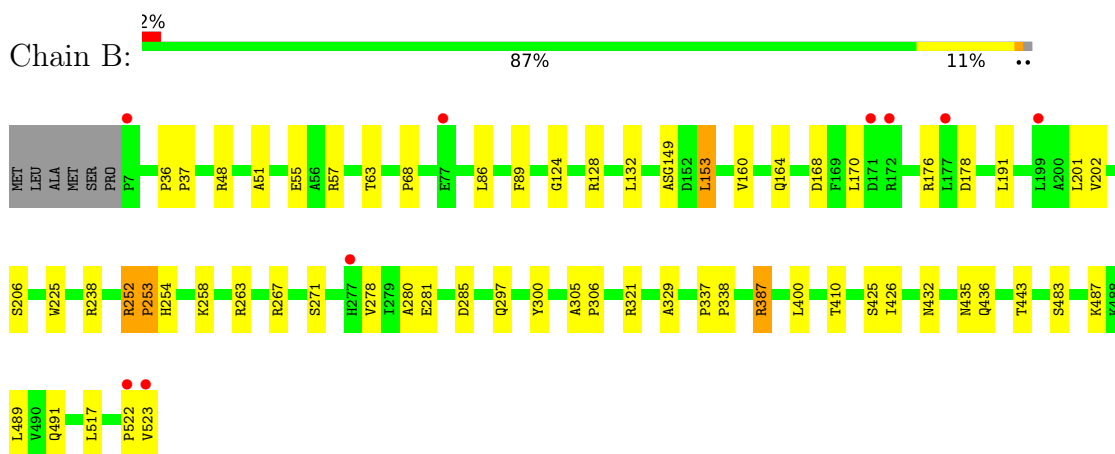
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

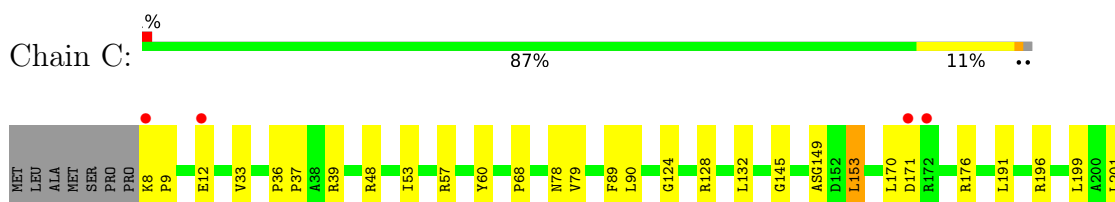
- Molecule 1: Putative histidine ammonia-lyase



- Molecule 1: Putative histidine ammonia-lyase

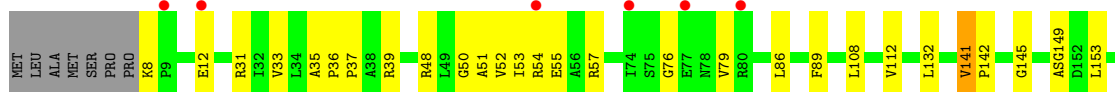
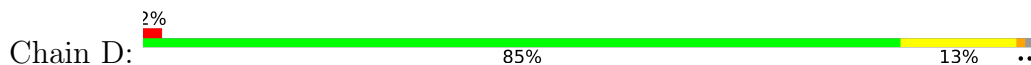


- Molecule 1: Putative histidine ammonia-lyase

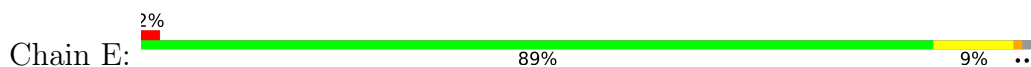




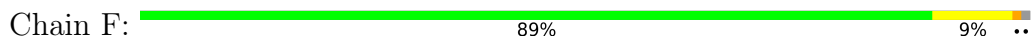
- Molecule 1: Putative histidine ammonia-lyase



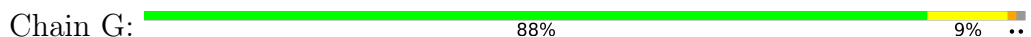
- Molecule 1: Putative histidine ammonia-lyase



- Molecule 1: Putative histidine ammonia-lyase

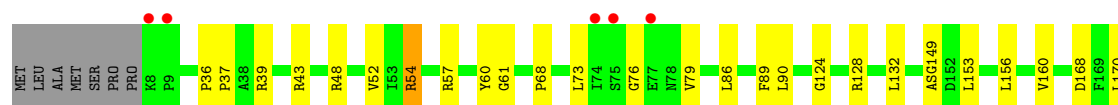
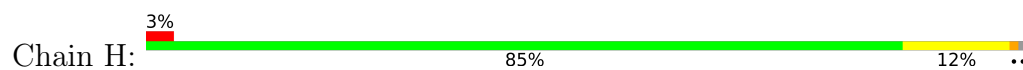


- Molecule 1: Putative histidine ammonia-lyase





● Molecule 1: Putative histidine ammonia-lyase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	87.59Å 155.05Å 164.04Å 90.00° 94.24° 90.00°	Depositor
Resolution (Å)	500.00 – 1.90 163.59 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.3 (500.00-1.90) 99.1 (163.59-1.90)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 1.89Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.172 , 0.196 0.172 , 0.196	Depositor DCC
R_{free} test set	17040 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	13.8	Xtrriage
Anisotropy	0.120	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 46.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	33846	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% 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: TCA, MDO

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	0.35	0/3863	0.85	7/5254 (0.1%)
1	B	0.35	0/3863	0.86	9/5254 (0.2%)
1	C	0.36	0/3855	0.87	9/5243 (0.2%)
1	D	0.36	0/3855	0.86	7/5243 (0.1%)
1	E	0.36	0/3855	0.85	6/5243 (0.1%)
1	F	0.36	0/3855	0.86	8/5243 (0.2%)
1	G	0.36	0/3855	0.86	9/5243 (0.2%)
1	H	0.35	0/3855	0.84	7/5243 (0.1%)
All	All	0.36	0/30856	0.86	62/41966 (0.1%)

There are no bond length outliers.

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	252	ARG	CA-C-N	7.10	128.72	119.84
1	F	252	ARG	C-N-CA	7.10	128.72	119.84
1	E	252	ARG	CA-C-N	7.08	128.69	119.84
1	E	252	ARG	C-N-CA	7.08	128.69	119.84
1	G	425	SER	N-CA-C	6.64	119.34	111.71
1	H	252	ARG	CA-C-N	6.62	128.12	119.84
1	H	252	ARG	C-N-CA	6.62	128.12	119.84
1	A	252	ARG	CA-C-N	6.41	127.86	119.84
1	A	252	ARG	C-N-CA	6.41	127.86	119.84
1	C	279	ILE	N-CA-C	6.37	117.12	110.62
1	G	252	ARG	CA-C-N	6.21	127.61	119.84
1	G	252	ARG	C-N-CA	6.21	127.61	119.84
1	E	425	SER	N-CA-C	6.17	118.81	111.71
1	C	252	ARG	CA-C-N	6.15	127.53	119.84
1	C	252	ARG	C-N-CA	6.15	127.53	119.84
1	H	253	PRO	N-CA-C	6.12	125.07	112.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	300	TYR	N-CA-C	6.06	117.89	111.28
1	D	425	SER	N-CA-C	6.04	118.66	111.71
1	B	254	HIS	N-CA-C	-5.97	102.12	109.65
1	H	425	SER	N-CA-C	5.97	118.56	111.33
1	D	252	ARG	CA-C-N	5.96	127.29	119.84
1	D	252	ARG	C-N-CA	5.96	127.29	119.84
1	A	253	PRO	N-CA-C	5.95	124.72	112.47
1	G	387	ARG	N-CA-C	5.86	119.32	111.24
1	F	253	PRO	N-CA-C	5.85	124.53	112.47
1	C	425	SER	N-CA-C	5.85	118.44	111.71
1	E	400	LEU	N-CA-C	-5.82	105.02	111.71
1	G	300	TYR	N-CA-C	5.81	117.61	111.28
1	D	253	PRO	N-CA-C	5.71	124.23	112.47
1	B	252	ARG	CA-C-N	5.70	126.97	119.84
1	B	252	ARG	C-N-CA	5.70	126.97	119.84
1	H	300	TYR	N-CA-C	5.61	118.16	111.71
1	B	253	PRO	N-CA-C	5.55	123.91	112.47
1	B	206	SER	N-CA-C	5.55	117.33	111.28
1	D	300	TYR	N-CA-C	5.54	118.08	111.71
1	A	425	SER	N-CA-C	5.54	118.84	111.75
1	C	253	PRO	N-CA-C	5.54	123.89	112.47
1	D	206	SER	N-CA-C	5.53	117.31	111.28
1	G	171	ASP	N-CA-C	-5.52	102.29	110.46
1	G	253	PRO	N-CA-C	5.52	123.84	112.47
1	B	300	TYR	N-CA-C	5.49	118.02	111.71
1	B	387	ARG	N-CA-C	5.48	118.80	111.24
1	F	206	SER	N-CA-C	5.43	117.20	111.28
1	F	425	SER	N-CA-C	5.42	117.94	111.71
1	H	387	ARG	N-CA-C	5.42	118.81	111.17
1	B	425	SER	N-CA-C	5.37	118.63	111.75
1	E	171	ASP	N-CA-C	-5.37	102.81	110.59
1	C	153	LEU	N-CA-C	5.33	116.78	111.07
1	C	171	ASP	N-CA-C	-5.31	102.90	110.59
1	C	342	VAL	N-CA-C	-5.30	104.85	109.19
1	E	253	PRO	N-CA-C	5.27	123.32	112.47
1	B	153	LEU	N-CA-C	5.26	116.69	111.07
1	F	171	ASP	N-CA-C	-5.22	103.02	110.59
1	G	440	SER	N-CA-C	5.20	118.09	111.69
1	H	206	SER	N-CA-C	5.17	116.92	111.28
1	F	387	ARG	N-CA-C	5.17	118.38	111.24
1	A	400	LEU	N-CA-C	-5.13	105.81	111.71
1	D	141	VAL	N-CA-C	5.12	113.71	107.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	387	ARG	N-CA-C	5.11	118.30	111.24
1	C	206	SER	N-CA-C	5.11	117.52	111.33
1	G	386	ASN	N-CA-C	5.10	118.64	112.93
1	A	300	TYR	N-CA-C	5.08	117.48	111.33

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	3814	0	3859	39	0
1	B	3814	0	3859	41	0
1	C	3807	0	3851	42	0
1	D	3807	0	3851	45	0
1	E	3807	0	3851	36	0
1	F	3807	0	3851	36	0
1	G	3807	0	3851	32	0
1	H	3807	0	3851	53	0
2	A	11	0	7	0	0
2	B	11	0	7	0	0
2	C	11	0	7	1	0
2	D	11	0	7	0	0
2	E	11	0	7	0	0
2	F	11	0	7	1	0
2	G	11	0	7	1	0
2	H	11	0	7	1	0
3	A	374	0	0	3	0
3	B	394	0	0	4	0
3	C	415	0	0	6	0
3	D	400	0	0	4	0
3	E	392	0	0	5	0
3	F	486	0	0	5	0
3	G	435	0	0	2	0
3	H	392	0	0	4	0
All	All	33846	0	30880	289	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 5.

All (289) 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:F:153:LEU:HD22	1:F:202:VAL:HG12	1.60	0.82
1:D:153:LEU:HD22	1:D:202:VAL:HG12	1.67	0.77
1:B:153:LEU:HD22	1:B:202:VAL:HG12	1.67	0.77
1:A:153:LEU:HD22	1:A:202:VAL:HG12	1.71	0.72
1:B:487:LYS:O	1:B:491:GLN:HG3	1.93	0.68
1:C:153:LEU:HD22	1:C:202:VAL:HG12	1.74	0.68
1:H:153:LEU:HD22	1:H:202:VAL:HG12	1.76	0.68
1:H:61:GLY:HA3	1:H:199:LEU:HD21	1.76	0.68
1:F:171:ASP:OD2	1:F:175:THR:HB	1.95	0.67
1:H:214:VAL:HB	1:H:450:ARG:NH2	2.09	0.67
1:A:68:PRO:HG3	1:A:435:ASN:HB2	1.77	0.67
1:B:51:ALA:O	1:B:55:GLU:HG3	1.95	0.66
1:H:36:PRO:HB2	1:H:37:PRO:HD3	1.77	0.66
1:A:495:GLU:HG3	1:A:496:GLN:HE21	1.60	0.66
1:C:487:LYS:O	1:C:491:GLN:HG3	1.96	0.65
1:B:258:LYS:HD2	3:B:3514:HOH:O	1.97	0.64
1:E:153:LEU:HD22	1:E:202:VAL:HG12	1.78	0.64
1:F:68:PRO:HG3	1:F:435:ASN:HB2	1.81	0.62
1:F:283:ARG:HD3	3:F:5119:HOH:O	2.00	0.61
1:A:280:ALA:O	1:D:57:ARG:HD2	2.00	0.60
1:C:176:ARG:HD2	3:C:3285:HOH:O	1.99	0.60
1:A:271:SER:HB2	1:A:483:SER:HB3	1.84	0.60
1:G:214:VAL:HB	1:G:450:ARG:NH2	2.16	0.60
1:F:426:ILE:HD13	3:G:3571:HOH:O	2.01	0.60
1:G:271:SER:HB2	1:G:483:SER:HB3	1.83	0.60
1:E:51:ALA:O	1:E:55:GLU:HG3	2.02	0.60
1:A:80:ARG:NH1	1:A:80:ARG:HG3	2.17	0.59
1:D:173:ASP:HB2	1:D:175:THR:HG23	1.85	0.59
1:G:487:LYS:O	1:G:491:GLN:HG3	2.01	0.59
1:B:124:GLY:O	1:B:128:ARG:HG2	2.03	0.59
1:G:39:ARG:HD2	1:G:43:ARG:NH2	2.17	0.59
1:G:53:ILE:HD13	1:G:196:ARG:HD2	1.85	0.58
1:G:153:LEU:HD22	1:G:202:VAL:HG12	1.84	0.58
1:B:238:ARG:HH21	1:B:387:ARG:HH21	1.50	0.58
1:D:50:GLY:O	1:D:54:ARG:HG3	2.04	0.58
1:C:68:PRO:HG3	1:C:435:ASN:HB2	1.85	0.57
1:A:426:ILE:HD13	3:D:3398:HOH:O	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:432:ASN:HB2	1:B:436:GLN:HE21	1.69	0.57
1:H:487:LYS:O	1:H:491:GLN:HG3	2.05	0.57
1:A:80:ARG:HG3	1:A:80:ARG:HH11	1.70	0.57
1:E:132:LEU:C	1:E:132:LEU:HD13	2.29	0.56
1:H:271:SER:HB2	1:H:483:SER:HB3	1.86	0.56
1:C:124:GLY:O	1:C:128:ARG:HG2	2.05	0.56
1:H:171:ASP:OD2	1:H:175:THR:HB	2.06	0.56
1:H:176:ARG:HD2	3:H:3379:HOH:O	2.05	0.55
1:B:57:ARG:HD2	1:C:280:ALA:O	2.07	0.55
1:F:36:PRO:HB2	1:F:37:PRO:HD3	1.89	0.55
1:F:225:TRP:CE2	1:F:517:LEU:HD22	2.42	0.55
1:G:132:LEU:HD13	1:G:132:LEU:C	2.32	0.55
1:H:297:GLN:HG3	3:H:2410:HOH:O	2.06	0.55
1:A:51:ALA:O	1:A:55:GLU:HG3	2.08	0.54
1:D:225:TRP:CE2	1:D:517:LEU:HD22	2.42	0.54
1:H:132:LEU:C	1:H:132:LEU:HD13	2.32	0.54
1:A:225:TRP:CE2	1:A:517:LEU:HD22	2.43	0.54
1:B:68:PRO:HG3	1:B:435:ASN:HB2	1.89	0.54
1:H:39:ARG:HG3	1:H:39:ARG:HH11	1.73	0.54
1:F:387:ARG:HD3	3:F:5133:HOH:O	2.06	0.54
3:A:3436:HOH:O	1:D:426:ILE:HD13	2.08	0.54
1:D:52:VAL:HG13	1:D:57:ARG:HB2	1.88	0.54
1:D:132:LEU:HD13	1:D:132:LEU:C	2.32	0.54
1:H:225:TRP:CE2	1:H:517:LEU:HD22	2.43	0.54
1:F:271:SER:HB2	1:F:483:SER:HB3	1.90	0.53
1:C:271:SER:HB2	1:C:483:SER:HB3	1.90	0.53
1:E:225:TRP:CE2	1:E:517:LEU:HD22	2.44	0.53
1:A:252:ARG:HA	1:D:329:ALA:HB1	1.90	0.53
1:A:132:LEU:C	1:A:132:LEU:HD13	2.34	0.53
1:B:191:LEU:HD21	1:B:201:LEU:CD1	2.39	0.52
1:D:36:PRO:HB2	1:D:37:PRO:HD3	1.90	0.52
1:E:489:LEU:HD23	1:E:489:LEU:C	2.34	0.52
1:E:487:LYS:O	1:E:491:GLN:HG3	2.10	0.52
1:G:372:LEU:O	1:G:376:GLN:HG3	2.09	0.52
3:F:3660:HOH:O	1:G:426:ILE:HD13	2.09	0.52
1:C:132:LEU:C	1:C:132:LEU:HD13	2.34	0.52
1:A:57:ARG:HD2	1:D:280:ALA:O	2.10	0.51
1:B:489:LEU:HD23	1:B:489:LEU:C	2.35	0.51
1:G:225:TRP:CE2	1:G:522:PRO:HD3	2.45	0.51
1:A:78:ASN:HB3	1:B:400:LEU:HD11	1.92	0.51
1:B:321:ARG:HH21	1:C:321:ARG:HH21	1.58	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:PRO:HB2	1:C:37:PRO:HD3	1.91	0.51
1:E:280:ALA:O	1:H:57:ARG:HD2	2.09	0.51
1:E:283:ARG:HD3	3:H:5485:HOH:O	2.10	0.51
1:H:214:VAL:HB	1:H:450:ARG:HH21	1.74	0.51
1:D:39:ARG:HG3	3:D:5784:HOH:O	2.10	0.51
1:B:271:SER:HB2	1:B:483:SER:HB3	1.93	0.51
1:D:12:GLU:HG2	1:D:35:ALA:HB2	1.92	0.51
1:D:271:SER:HB2	1:D:483:SER:HB3	1.93	0.51
1:E:57:ARG:HD2	1:H:280:ALA:O	2.11	0.51
1:A:372:LEU:O	1:A:376:GLN:HG3	2.10	0.51
1:E:271:SER:HB2	1:E:483:SER:HB3	1.93	0.51
1:E:263:ARG:O	1:E:267:ARG:HG2	2.10	0.51
1:A:52:VAL:HG13	1:A:57:ARG:HB2	1.92	0.51
1:E:329:ALA:HB1	1:H:252:ARG:HA	1.93	0.51
1:H:489:LEU:C	1:H:489:LEU:HD23	2.36	0.51
1:A:80:ARG:HH11	1:A:80:ARG:CG	2.24	0.51
1:G:124:GLY:O	1:G:128:ARG:HG2	2.11	0.51
1:H:283:ARG:HD3	3:H:5169:HOH:O	2.11	0.50
1:A:495:GLU:HG3	1:A:496:GLN:NE2	2.26	0.50
1:B:132:LEU:HD13	1:B:132:LEU:C	2.36	0.50
1:E:152:ASP:CG	1:E:207:ALA:HB3	2.37	0.50
1:G:523:VAL:OXT	1:G:523:VAL:HG12	2.10	0.50
1:H:170:LEU:HD23	1:H:176:ARG:HG2	1.94	0.50
1:C:225:TRP:CE2	1:C:517:LEU:HD22	2.46	0.50
1:C:523:VAL:OXT	1:C:523:VAL:HG12	2.11	0.50
1:E:176:ARG:HD2	3:E:3308:HOH:O	2.11	0.50
1:H:68:PRO:HG3	1:H:435:ASN:HB2	1.94	0.50
1:F:124:GLY:O	1:F:128:ARG:HG2	2.12	0.50
1:B:329:ALA:HB1	1:C:252:ARG:HA	1.94	0.49
1:C:48:ARG:HH11	1:C:48:ARG:HG2	1.77	0.49
1:E:53:ILE:HD13	1:E:196:ARG:HD2	1.94	0.49
1:E:124:GLY:O	1:E:128:ARG:HG2	2.12	0.49
1:G:54:ARG:HD2	3:G:2686:HOH:O	2.12	0.49
1:H:124:GLY:O	1:H:128:ARG:HG2	2.12	0.49
1:B:280:ALA:O	1:C:57:ARG:HD2	2.13	0.49
1:A:184:ARG:HG2	1:A:184:ARG:HH11	1.78	0.49
1:B:426:ILE:HD13	3:C:3493:HOH:O	2.12	0.49
1:B:86:LEU:HA	1:B:89:PHE:CE2	2.47	0.49
1:B:170:LEU:CD2	1:B:176:ARG:HG2	2.43	0.49
1:A:321:ARG:HH21	1:D:321:ARG:HH21	1.59	0.49
1:B:225:TRP:CE2	1:B:517:LEU:HD22	2.48	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:160:VAL:O	1:G:164:GLN:HG3	2.13	0.49
1:B:523:VAL:OXT	1:B:523:VAL:HG12	2.13	0.49
1:G:36:PRO:N	1:G:37:PRO:HD2	2.28	0.49
1:F:53:ILE:HD13	1:F:196:ARG:HD2	1.95	0.48
1:A:329:ALA:HB1	1:D:252:ARG:HA	1.95	0.48
1:A:487:LYS:O	1:A:491:GLN:HG3	2.13	0.48
1:C:225:TRP:CD2	1:C:522:PRO:HG3	2.48	0.48
1:G:60:TYR:OH	2:G:701:TCA:H2	2.14	0.48
1:A:170:LEU:HD23	1:A:176:ARG:HG2	1.95	0.48
3:B:3548:HOH:O	1:C:426:ILE:HD13	2.13	0.48
1:D:169:PHE:CD2	1:D:182:GLY:HA3	2.48	0.48
1:F:181:GLU:OE1	1:F:184:ARG:NH1	2.47	0.48
1:A:176:ARG:HD2	3:A:3332:HOH:O	2.14	0.48
1:B:170:LEU:HD23	1:B:176:ARG:HG2	1.96	0.48
1:F:57:ARG:HD2	1:G:280:ALA:O	2.14	0.48
1:C:60:TYR:OH	2:C:701:TCA:H2	2.14	0.47
1:C:263:ARG:O	1:C:267:ARG:HG2	2.13	0.47
1:C:489:LEU:C	1:C:489:LEU:HD23	2.38	0.47
1:A:124:GLY:O	1:A:128:ARG:HG2	2.14	0.47
1:D:48:ARG:NH2	1:D:338:PRO:O	2.47	0.47
1:F:489:LEU:C	1:F:489:LEU:HD23	2.39	0.47
1:D:191:LEU:HD21	1:D:201:LEU:CD1	2.45	0.47
1:E:12:GLU:HA	1:E:33:VAL:HG13	1.96	0.47
1:E:384:ARG:HD2	3:E:3602:HOH:O	2.15	0.47
1:H:372:LEU:O	1:H:376:GLN:HG3	2.15	0.47
1:B:168:ASP:HB2	1:B:176:ARG:HH21	1.80	0.47
1:H:54:ARG:HG2	1:H:54:ARG:HH11	1.80	0.47
1:E:80:ARG:HG2	3:E:4938:HOH:O	2.15	0.47
1:A:36:PRO:N	1:A:37:PRO:HD2	2.29	0.47
1:B:36:PRO:HB2	1:B:37:PRO:HD3	1.96	0.46
1:B:160:VAL:O	1:B:164:GLN:HG3	2.15	0.46
1:D:51:ALA:O	1:D:55:GLU:HG3	2.15	0.46
1:F:171:ASP:C	1:F:171:ASP:OD1	2.58	0.46
1:F:436:GLN:HG2	1:G:300:TYR:CZ	2.51	0.46
1:G:489:LEU:HD23	1:G:489:LEU:C	2.40	0.46
1:B:252:ARG:HA	1:C:329:ALA:HB1	1.96	0.46
1:H:156:LEU:O	1:H:160:VAL:HG23	2.15	0.46
1:A:7:PRO:O	1:A:8:LYS:C	2.59	0.46
1:B:436:GLN:HG2	1:C:300:TYR:CZ	2.51	0.46
1:E:145:GLY:HA2	1:F:410:THR:HG23	1.97	0.46
1:A:263:ARG:O	1:A:267:ARG:HG2	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:252:ARG:HA	1:G:329:ALA:HB1	1.97	0.46
1:F:329:ALA:HB1	1:G:252:ARG:HA	1.98	0.46
1:H:168:ASP:HB2	1:H:176:ARG:HH21	1.81	0.46
1:A:489:LEU:C	1:A:489:LEU:HD23	2.40	0.45
1:B:297:GLN:HG3	3:B:3097:HOH:O	2.16	0.45
1:H:86:LEU:HA	1:H:89:PHE:CE2	2.50	0.45
1:A:160:VAL:O	1:A:164:GLN:HG3	2.16	0.45
1:C:225:TRP:CE2	1:C:522:PRO:HG3	2.51	0.45
3:E:3348:HOH:O	1:H:426:ILE:HD13	2.17	0.45
1:H:238:ARG:HH11	1:H:387:ARG:NH2	2.15	0.45
1:C:53:ILE:HD13	1:C:196:ARG:HD2	1.98	0.45
1:H:76:GLY:HA2	1:H:79:VAL:HG23	1.97	0.45
1:C:170:LEU:HD23	1:C:176:ARG:HG2	1.98	0.45
1:D:211:ILE:HD13	1:D:447:ARG:HG3	1.98	0.45
1:G:225:TRP:CE2	1:G:517:LEU:HD22	2.52	0.45
1:H:199:LEU:HD12	1:H:199:LEU:N	2.32	0.45
1:G:90:LEU:HD13	1:G:153:LEU:HB3	1.99	0.45
1:A:146:THR:HG22	3:A:2274:HOH:O	2.16	0.45
1:B:225:TRP:CE2	1:B:522:PRO:HD3	2.52	0.45
1:D:199:LEU:O	1:D:203:ASN:HB2	2.17	0.45
1:E:79:VAL:HG11	1:E:196:ARG:HD3	1.99	0.45
1:D:489:LEU:C	1:D:489:LEU:HD23	2.42	0.44
1:H:184:ARG:HG2	1:H:184:ARG:HH11	1.82	0.44
1:C:410:THR:HG23	1:D:145:GLY:HA2	1.99	0.44
1:C:491:GLN:O	1:C:495:GLU:HG3	2.17	0.44
1:E:436:GLN:HG2	1:H:300:TYR:CZ	2.52	0.44
1:A:86:LEU:HA	1:A:89:PHE:CE2	2.53	0.44
1:D:12:GLU:CG	1:D:35:ALA:HB2	2.47	0.44
1:F:132:LEU:C	1:F:132:LEU:HD13	2.42	0.44
1:D:433:ALA:O	1:D:434:ALA:HB3	2.17	0.44
1:E:78:ASN:HB3	1:F:400:LEU:HD21	1.99	0.44
1:D:12:GLU:HA	1:D:33:VAL:HG13	1.99	0.44
1:B:238:ARG:HH21	1:B:387:ARG:NH2	2.15	0.44
1:F:321:ARG:HH21	1:G:321:ARG:HH21	1.64	0.44
1:G:395:ARG:CZ	1:G:501:GLU:HG2	2.48	0.44
1:H:225:TRP:CE2	1:H:522:PRO:HD3	2.53	0.44
1:D:372:LEU:O	1:D:376:GLN:HG3	2.17	0.44
1:E:497:PHE:HA	1:E:498:PRO:HD3	1.85	0.44
1:F:242:GLU:HB3	3:F:1183:HOH:O	2.18	0.44
1:C:78:ASN:HB3	1:D:400:LEU:HD21	2.00	0.43
1:C:90:LEU:HD13	1:C:153:LEU:HB3	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:171:ASP:OD1	1:G:171:ASP:C	2.60	0.43
1:A:125:THR:HG23	1:A:201:LEU:HD11	2.01	0.43
1:C:48:ARG:HG2	1:C:48:ARG:NH1	2.33	0.43
1:C:214:VAL:HG13	3:C:4020:HOH:O	2.18	0.43
1:A:170:LEU:CD2	1:A:176:ARG:HG2	2.49	0.43
1:C:12:GLU:HA	1:C:33:VAL:HG13	2.00	0.43
1:C:191:LEU:HD21	1:C:201:LEU:CD1	2.48	0.43
1:D:335:VAL:HG11	3:D:2240:HOH:O	2.17	0.43
1:G:337:PRO:HA	1:G:338:PRO:HD3	1.92	0.43
1:H:60:TYR:OH	2:H:701:TCA:H2	2.19	0.43
1:D:79:VAL:HG21	3:D:5014:HOH:O	2.19	0.43
1:E:80:ARG:HB3	1:E:80:ARG:HH11	1.84	0.43
1:F:60:TYR:OH	2:F:701:TCA:H2	2.17	0.43
1:A:184:ARG:HG2	1:A:184:ARG:NH1	2.33	0.43
1:D:53:ILE:HD13	1:D:196:ARG:HD2	2.00	0.43
1:D:177:LEU:HD21	1:D:185:ARG:NH1	2.33	0.43
1:F:305:ALA:N	1:F:306:PRO:CD	2.82	0.43
1:H:52:VAL:HG13	1:H:57:ARG:HB2	2.01	0.43
1:C:145:GLY:HA2	1:D:410:THR:HG23	2.01	0.42
1:D:225:TRP:CD2	1:D:517:LEU:HD22	2.53	0.42
1:F:225:TRP:CD2	1:F:517:LEU:HD22	2.54	0.42
1:E:321:ARG:HH21	1:H:321:ARG:HH21	1.67	0.42
1:E:48:ARG:HH11	1:E:48:ARG:HG2	1.84	0.42
1:E:305:ALA:HB3	1:E:306:PRO:HD3	2.02	0.42
1:H:497:PHE:HA	1:H:498:PRO:HD3	1.88	0.42
1:C:79:VAL:HG11	1:C:196:ARG:HD3	2.02	0.42
1:G:214:VAL:HB	1:G:450:ARG:HH21	1.82	0.42
1:H:238:ARG:NH1	1:H:387:ARG:NH2	2.67	0.42
1:H:191:LEU:HD21	1:H:201:LEU:CD1	2.50	0.42
1:D:184:ARG:HG2	1:D:184:ARG:HH11	1.84	0.42
1:H:90:LEU:HD13	1:H:153:LEU:HB3	2.01	0.42
1:H:171:ASP:C	1:H:171:ASP:OD1	2.62	0.42
1:H:48:ARG:O	1:H:52:VAL:HG23	2.20	0.42
1:H:184:ARG:HG2	1:H:184:ARG:NH1	2.35	0.42
1:H:263:ARG:O	1:H:267:ARG:HG2	2.20	0.42
1:B:285:ASP:C	1:B:285:ASP:OD2	2.63	0.41
1:C:394:HIS:HE1	3:C:2881:HOH:O	2.02	0.41
1:D:141:VAL:HA	1:D:142:PRO:HD3	1.97	0.41
1:E:252:ARG:HA	1:H:329:ALA:HB1	2.02	0.41
1:F:372:LEU:O	1:F:376:GLN:HG3	2.20	0.41
1:B:48:ARG:NH2	1:B:338:PRO:O	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:PRO:HG3	1:B:435:ASN:CB	2.50	0.41
1:H:48:ARG:NH2	1:H:338:PRO:O	2.52	0.41
1:G:263:ARG:O	1:G:267:ARG:HG2	2.20	0.41
1:A:279:ILE:HD11	1:D:346:HIS:CE1	2.55	0.41
1:D:285:ASP:OD2	1:D:285:ASP:C	2.63	0.41
1:E:79:VAL:HG21	3:E:2045:HOH:O	2.20	0.41
1:H:170:LEU:CD2	1:H:176:ARG:HG2	2.49	0.41
1:B:178:ASP:OD2	1:B:178:ASP:C	2.63	0.41
1:C:8:LYS:HA	1:C:9:PRO:HD3	1.94	0.41
1:C:335:VAL:HG11	3:C:1256:HOH:O	2.20	0.41
1:E:410:THR:HG23	1:F:145:GLY:HA2	2.02	0.41
1:H:39:ARG:HD3	1:H:43:ARG:HH21	1.86	0.41
1:A:305:ALA:N	1:A:306:PRO:CD	2.84	0.41
1:H:305:ALA:N	1:H:306:PRO:CD	2.84	0.41
1:C:199:LEU:O	1:C:203:ASN:HB2	2.21	0.41
1:G:211:ILE:HD13	1:G:447:ARG:HG3	2.03	0.41
1:H:39:ARG:O	1:H:43:ARG:HG3	2.20	0.41
1:A:79:VAL:HG11	1:A:196:ARG:HD3	2.03	0.41
1:A:145:GLY:HA2	1:B:410:THR:HG23	2.03	0.41
1:B:63:THR:HG22	3:B:5022:HOH:O	2.20	0.41
1:B:278:VAL:HB	1:B:281:GLU:HG3	2.02	0.41
1:B:337:PRO:HA	1:B:338:PRO:HD3	1.93	0.41
1:D:225:TRP:CE2	1:D:522:PRO:HD3	2.56	0.41
1:E:288:ASP:O	1:H:73:LEU:HD12	2.21	0.41
1:F:79:VAL:HG11	1:F:196:ARG:HD3	2.02	0.41
1:F:280:ALA:O	1:G:57:ARG:HD2	2.20	0.41
1:F:285:ASP:OD2	1:F:285:ASP:C	2.63	0.41
1:G:78:ASN:HB3	1:H:400:LEU:HD21	2.03	0.41
1:B:305:ALA:N	1:B:306:PRO:CD	2.84	0.41
1:F:68:PRO:HG3	1:F:435:ASN:CB	2.50	0.41
1:F:335:VAL:HG11	3:F:1411:HOH:O	2.22	0.40
1:B:263:ARG:O	1:B:267:ARG:HG2	2.21	0.40
1:D:86:LEU:HA	1:D:89:PHE:CE2	2.56	0.40
1:D:281:GLU:OE1	1:D:281:GLU:HA	2.22	0.40
1:E:100:TRP:CZ2	1:E:172:ARG:HG2	2.55	0.40
1:F:89:PHE:CD1	1:F:89:PHE:C	2.99	0.40
1:C:39:ARG:NH1	3:C:5446:HOH:O	2.54	0.40
1:E:48:ARG:HG2	1:E:48:ARG:NH1	2.37	0.40
1:E:160:VAL:O	1:E:164:GLN:HG3	2.22	0.40
1:C:372:LEU:O	1:C:376:GLN:HG3	2.21	0.40
1:E:436:GLN:HG2	1:H:300:TYR:CE2	2.57	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:281:GLU:OE1	1:F:281:GLU:HA	2.22	0.40
1:C:89:PHE:CD1	1:C:89:PHE:C	3.00	0.40
1:D:8:LYS:CG	1:D:31:ARG:HG3	2.51	0.40
1:D:76:GLY:HA2	1:D:79:VAL:HG23	2.04	0.40
1:D:108:LEU:O	1:D:112:VAL:HG23	2.21	0.40
1:F:424:ALA:HB2	1:F:448:LEU:HD12	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	510/521 (98%)	499 (98%)	9 (2%)	2 (0%)	30	22
1	B	510/521 (98%)	504 (99%)	5 (1%)	1 (0%)	43	36
1	C	509/521 (98%)	503 (99%)	5 (1%)	1 (0%)	43	36
1	D	509/521 (98%)	499 (98%)	9 (2%)	1 (0%)	43	36
1	E	509/521 (98%)	503 (99%)	5 (1%)	1 (0%)	43	36
1	F	509/521 (98%)	501 (98%)	7 (1%)	1 (0%)	43	36
1	G	509/521 (98%)	502 (99%)	6 (1%)	1 (0%)	43	36
1	H	509/521 (98%)	500 (98%)	8 (2%)	1 (0%)	43	36
All	All	4074/4168 (98%)	4011 (98%)	54 (1%)	9 (0%)	43	36

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	253	PRO
1	E	253	PRO
1	A	253	PRO
1	C	253	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	253	PRO
1	H	253	PRO
1	A	8	LYS
1	B	253	PRO
1	D	253	PRO

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	384/389 (99%)	382 (100%)	2 (0%)	81	84
1	B	384/389 (99%)	383 (100%)	1 (0%)	86	88
1	C	383/389 (98%)	382 (100%)	1 (0%)	86	88
1	D	383/389 (98%)	382 (100%)	1 (0%)	86	88
1	E	383/389 (98%)	381 (100%)	2 (0%)	81	84
1	F	383/389 (98%)	381 (100%)	2 (0%)	81	84
1	G	383/389 (98%)	382 (100%)	1 (0%)	86	88
1	H	383/389 (98%)	381 (100%)	2 (0%)	81	84
All	All	3066/3112 (98%)	3054 (100%)	12 (0%)	84	87

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	ARG
1	A	443	THR
1	B	443	THR
1	C	443	THR
1	D	443	THR
1	E	80	ARG
1	E	443	THR
1	F	242	GLU
1	F	443	THR
1	G	443	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	54	ARG
1	H	443	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	164	GLN
1	A	195	HIS
1	A	353	GLN
1	A	435	ASN
1	A	491	GLN
1	A	496	GLN
1	B	164	GLN
1	B	189	GLN
1	B	353	GLN
1	B	435	ASN
1	B	436	GLN
1	B	520	GLN
1	C	164	GLN
1	C	189	GLN
1	C	277	HIS
1	C	394	HIS
1	C	435	ASN
1	D	164	GLN
1	D	394	HIS
1	D	435	ASN
1	D	436	GLN
1	D	491	GLN
1	D	496	GLN
1	D	519	GLN
1	E	164	GLN
1	E	436	GLN
1	E	520	GLN
1	F	164	GLN
1	F	195	HIS
1	F	435	ASN
1	F	491	GLN
1	G	164	GLN
1	G	435	ASN
1	H	394	HIS
1	H	508	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](#)

8 non-standard protein/DNA/RNA residues 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
1	MDO	B	149	1	11,13,14	2.58	5 (45%)	15,18,20	2.48	5 (33%)
1	MDO	H	149	1	11,13,14	2.46	4 (36%)	15,18,20	2.60	5 (33%)
1	MDO	G	149	1	11,13,14	2.43	4 (36%)	15,18,20	2.64	5 (33%)
1	MDO	C	149	1	11,13,14	2.43	4 (36%)	15,18,20	2.58	5 (33%)
1	MDO	D	149	1	11,13,14	2.46	4 (36%)	15,18,20	2.62	6 (40%)
1	MDO	E	149	1	11,13,14	2.42	4 (36%)	15,18,20	2.59	5 (33%)
1	MDO	F	149	1	11,13,14	2.43	4 (36%)	15,18,20	2.66	5 (33%)
1	MDO	A	149	1	11,13,14	2.43	4 (36%)	15,18,20	2.54	5 (33%)

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
1	MDO	B	149	1	-	0/4/23/24	0/1/1/1
1	MDO	H	149	1	-	1/4/23/24	0/1/1/1
1	MDO	G	149	1	-	1/4/23/24	0/1/1/1
1	MDO	C	149	1	-	1/4/23/24	0/1/1/1
1	MDO	D	149	1	-	0/4/23/24	0/1/1/1
1	MDO	E	149	1	-	1/4/23/24	0/1/1/1
1	MDO	F	149	1	-	1/4/23/24	0/1/1/1
1	MDO	A	149	1	-	0/4/23/24	0/1/1/1

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	149	MDO	O2-C2	5.43	1.34	1.23
1	H	149	MDO	O2-C2	5.28	1.33	1.23
1	D	149	MDO	O2-C2	5.25	1.33	1.23
1	C	149	MDO	O2-C2	5.24	1.33	1.23
1	F	149	MDO	O2-C2	5.19	1.33	1.23
1	E	149	MDO	O2-C2	5.14	1.33	1.23
1	A	149	MDO	O2-C2	5.14	1.33	1.23
1	G	149	MDO	O2-C2	5.09	1.33	1.23
1	B	149	MDO	C2-N3	-3.98	1.30	1.40
1	A	149	MDO	C2-N3	-3.86	1.31	1.40
1	E	149	MDO	C2-N3	-3.82	1.31	1.40
1	D	149	MDO	C2-N3	-3.73	1.31	1.40
1	G	149	MDO	C2-N3	-3.72	1.31	1.40
1	C	149	MDO	C2-N3	-3.70	1.31	1.40
1	H	149	MDO	C2-N3	-3.68	1.31	1.40
1	F	149	MDO	C2-N3	-3.67	1.31	1.40
1	C	149	MDO	CA2-N2	-3.02	1.33	1.39
1	G	149	MDO	CA2-N2	-2.97	1.34	1.39
1	B	149	MDO	CA2-N2	-2.95	1.34	1.39
1	E	149	MDO	CA2-N2	-2.93	1.34	1.39
1	A	149	MDO	CA2-N2	-2.91	1.34	1.39
1	F	149	MDO	CA2-C2	-2.80	1.37	1.43
1	H	149	MDO	CA2-C2	-2.68	1.37	1.43
1	H	149	MDO	CA2-N2	-2.66	1.34	1.39
1	D	149	MDO	CA2-C2	-2.63	1.38	1.43
1	E	149	MDO	CA2-C2	-2.59	1.38	1.43
1	F	149	MDO	CA2-N2	-2.57	1.34	1.39
1	G	149	MDO	CA2-C2	-2.57	1.38	1.43
1	D	149	MDO	CA2-N2	-2.52	1.34	1.39
1	B	149	MDO	CA2-C2	-2.51	1.38	1.43
1	A	149	MDO	CA2-C2	-2.42	1.38	1.43
1	C	149	MDO	CA2-C2	-2.34	1.38	1.43
1	B	149	MDO	C1-N3	-2.28	1.33	1.37

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	149	MDO	CA2-C2-N3	6.85	109.25	103.50
1	F	149	MDO	CA2-C2-N3	6.83	109.24	103.50
1	G	149	MDO	CA2-C2-N3	6.82	109.23	103.50
1	E	149	MDO	CA2-C2-N3	6.82	109.23	103.50
1	H	149	MDO	CA2-C2-N3	6.79	109.20	103.50
1	B	149	MDO	CA2-C2-N3	6.74	109.16	103.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	149	MDO	CA2-C2-N3	6.74	109.16	103.50
1	A	149	MDO	CA2-C2-N3	6.73	109.15	103.50
1	F	149	MDO	O2-C2-CA2	-4.67	128.04	131.02
1	G	149	MDO	O2-C2-CA2	-4.51	128.14	131.02
1	D	149	MDO	O2-C2-CA2	-4.39	128.22	131.02
1	H	149	MDO	O2-C2-CA2	-4.38	128.22	131.02
1	E	149	MDO	O2-C2-CA2	-4.30	128.28	131.02
1	C	149	MDO	O2-C2-CA2	-4.16	128.37	131.02
1	A	149	MDO	O2-C2-CA2	-4.09	128.41	131.02
1	D	149	MDO	C2-CA2-N2	-3.69	106.31	108.95
1	B	149	MDO	C2-CA2-N2	-3.66	106.33	108.95
1	A	149	MDO	C2-CA2-N2	-3.60	106.37	108.95
1	B	149	MDO	O2-C2-CA2	-3.57	128.74	131.02
1	C	149	MDO	C2-CA2-N2	-3.50	106.44	108.95
1	H	149	MDO	C2-CA2-N2	-3.49	106.45	108.95
1	F	149	MDO	C2-CA2-N2	-3.44	106.49	108.95
1	E	149	MDO	C2-CA2-N2	-3.42	106.50	108.95
1	G	149	MDO	C2-CA2-N2	-3.36	106.55	108.95
1	F	149	MDO	N3-C1-N2	-2.92	109.18	111.48
1	H	149	MDO	N3-C1-N2	-2.76	109.31	111.48
1	D	149	MDO	N3-C1-N2	-2.72	109.34	111.48
1	G	149	MDO	N3-C1-N2	-2.65	109.39	111.48
1	C	149	MDO	CA2-N2-C1	2.65	107.77	105.39
1	C	149	MDO	N3-C1-N2	-2.65	109.40	111.48
1	E	149	MDO	N3-C1-N2	-2.63	109.41	111.48
1	E	149	MDO	CA2-N2-C1	2.52	107.65	105.39
1	F	149	MDO	CA2-N2-C1	2.52	107.65	105.39
1	G	149	MDO	CA2-N2-C1	2.50	107.63	105.39
1	H	149	MDO	CA2-N2-C1	2.44	107.58	105.39
1	A	149	MDO	CA2-N2-C1	2.44	107.58	105.39
1	D	149	MDO	CA2-N2-C1	2.39	107.53	105.39
1	A	149	MDO	N3-C1-N2	-2.38	109.61	111.48
1	B	149	MDO	N3-C1-N2	-2.31	109.66	111.48
1	B	149	MDO	CA2-N2-C1	2.20	107.37	105.39
1	D	149	MDO	CA1-C1-N2	2.04	126.60	124.04

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	149	MDO	N2-C1-CA1-CB
1	E	149	MDO	N2-C1-CA1-CB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	F	149	MDO	N2-C1-CA1-CB
1	G	149	MDO	N2-C1-CA1-CB
1	H	149	MDO	N2-C1-CA1-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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	TCA	F	701	-	11,11,11	2.44	6 (54%)	13,13,13	0.50	0
2	TCA	B	701	-	11,11,11	2.46	7 (63%)	13,13,13	0.53	0
2	TCA	A	701	-	11,11,11	2.41	6 (54%)	13,13,13	0.49	0
2	TCA	G	701	-	11,11,11	2.45	7 (63%)	13,13,13	0.49	0
2	TCA	C	701	-	11,11,11	2.42	6 (54%)	13,13,13	0.52	0
2	TCA	E	701	-	11,11,11	2.43	7 (63%)	13,13,13	0.51	0
2	TCA	D	701	-	11,11,11	2.45	6 (54%)	13,13,13	0.51	0
2	TCA	H	701	-	11,11,11	2.42	6 (54%)	13,13,13	0.50	0

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	TCA	F	701	-	-	2/5/5/5	0/1/1/1
2	TCA	B	701	-	-	2/5/5/5	0/1/1/1
2	TCA	A	701	-	-	2/5/5/5	0/1/1/1
2	TCA	G	701	-	-	2/5/5/5	0/1/1/1
2	TCA	C	701	-	-	2/5/5/5	0/1/1/1
2	TCA	E	701	-	-	2/5/5/5	0/1/1/1
2	TCA	D	701	-	-	2/5/5/5	0/1/1/1
2	TCA	H	701	-	-	2/5/5/5	0/1/1/1

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	701	TCA	C33-C32	3.52	1.44	1.38
2	H	701	TCA	C33-C32	3.50	1.44	1.38
2	C	701	TCA	C33-C32	3.45	1.44	1.38
2	G	701	TCA	C33-C32	3.45	1.44	1.38
2	F	701	TCA	C33-C32	3.42	1.44	1.38
2	D	701	TCA	C33-C32	3.41	1.44	1.38
2	B	701	TCA	C33-C32	3.37	1.44	1.38
2	A	701	TCA	C33-C32	3.37	1.44	1.38
2	H	701	TCA	C32-C31	3.35	1.46	1.39
2	D	701	TCA	C32-C31	3.31	1.46	1.39
2	E	701	TCA	C32-C31	3.29	1.46	1.39
2	B	701	TCA	C32-C31	3.28	1.46	1.39
2	A	701	TCA	C32-C31	3.27	1.46	1.39
2	F	701	TCA	C32-C31	3.25	1.46	1.39
2	G	701	TCA	C32-C31	3.21	1.46	1.39
2	G	701	TCA	C35-C36	3.17	1.44	1.38
2	C	701	TCA	C32-C31	3.13	1.45	1.39
2	B	701	TCA	C35-C36	3.10	1.44	1.38
2	C	701	TCA	C35-C36	3.07	1.44	1.38
2	E	701	TCA	C35-C36	3.05	1.44	1.38
2	D	701	TCA	C35-C36	3.05	1.44	1.38
2	F	701	TCA	C35-C36	3.02	1.44	1.38
2	B	701	TCA	C35-C34	3.00	1.44	1.38
2	D	701	TCA	C36-C31	2.99	1.45	1.39
2	B	701	TCA	C36-C31	2.99	1.45	1.39
2	C	701	TCA	C35-C34	2.98	1.44	1.38
2	A	701	TCA	C35-C36	2.97	1.44	1.38
2	D	701	TCA	C35-C34	2.97	1.44	1.38
2	F	701	TCA	C36-C31	2.97	1.45	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	701	TCA	C35-C36	2.96	1.44	1.38
2	H	701	TCA	C35-C34	2.93	1.44	1.38
2	F	701	TCA	C35-C34	2.91	1.44	1.38
2	G	701	TCA	C36-C31	2.91	1.45	1.39
2	C	701	TCA	C36-C31	2.90	1.45	1.39
2	A	701	TCA	C35-C34	2.89	1.44	1.38
2	E	701	TCA	C35-C34	2.88	1.44	1.38
2	E	701	TCA	C36-C31	2.87	1.45	1.39
2	A	701	TCA	C36-C31	2.82	1.45	1.39
2	G	701	TCA	C34-C33	2.80	1.44	1.38
2	G	701	TCA	C35-C34	2.79	1.44	1.38
2	H	701	TCA	C36-C31	2.78	1.45	1.39
2	B	701	TCA	C34-C33	2.77	1.44	1.38
2	H	701	TCA	C34-C33	2.74	1.44	1.38
2	D	701	TCA	C34-C33	2.72	1.44	1.38
2	F	701	TCA	C34-C33	2.72	1.44	1.38
2	A	701	TCA	C34-C33	2.68	1.44	1.38
2	C	701	TCA	C34-C33	2.64	1.44	1.38
2	E	701	TCA	C34-C33	2.62	1.44	1.38
2	B	701	TCA	OXT-C1	-2.12	1.25	1.30
2	G	701	TCA	OXT-C1	-2.05	1.25	1.30
2	E	701	TCA	OXT-C1	-2.01	1.25	1.30

There are no bond angle outliers.

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	701	TCA	O-C1-C2-C3
2	F	701	TCA	O-C1-C2-C3
2	F	701	TCA	OXT-C1-C2-C3
2	B	701	TCA	O-C1-C2-C3
2	B	701	TCA	OXT-C1-C2-C3
2	E	701	TCA	O-C1-C2-C3
2	E	701	TCA	OXT-C1-C2-C3
2	G	701	TCA	OXT-C1-C2-C3
2	D	701	TCA	O-C1-C2-C3
2	H	701	TCA	O-C1-C2-C3
2	A	701	TCA	OXT-C1-C2-C3
2	D	701	TCA	OXT-C1-C2-C3
2	H	701	TCA	OXT-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	701	TCA	O-C1-C2-C3
2	C	701	TCA	OXT-C1-C2-C3
2	C	701	TCA	O-C1-C2-C3

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	701	TCA	1	0
2	G	701	TCA	1	0
2	C	701	TCA	1	0
2	H	701	TCA	1	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	514/521 (98%)	-0.09	17 (3%) 49 52	6, 14, 34, 54	0
1	B	514/521 (98%)	-0.23	9 (1%) 67 71	5, 13, 31, 49	0
1	C	513/521 (98%)	-0.31	6 (1%) 76 79	6, 12, 27, 48	0
1	D	513/521 (98%)	-0.15	11 (2%) 63 67	3, 14, 32, 50	0
1	E	513/521 (98%)	-0.25	9 (1%) 67 71	4, 13, 31, 50	0
1	F	513/521 (98%)	-0.42	2 (0%) 88 90	3, 11, 24, 43	0
1	G	513/521 (98%)	-0.37	2 (0%) 88 90	4, 11, 26, 46	0
1	H	513/521 (98%)	-0.12	14 (2%) 56 60	5, 14, 32, 49	0
All	All	4106/4168 (98%)	-0.24	70 (1%) 69 72	3, 13, 30, 54	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	523	VAL	6.6
1	B	523	VAL	6.1
1	F	523	VAL	6.0
1	H	523	VAL	6.0
1	A	285	ASP	6.0
1	A	523	VAL	5.9
1	C	523	VAL	5.4
1	E	523	VAL	5.0
1	B	277	HIS	5.0
1	D	277	HIS	4.9
1	G	523	VAL	4.9
1	A	7	PRO	4.9
1	B	7	PRO	4.8
1	H	277	HIS	4.3
1	F	277	HIS	4.1
1	A	289	ILE	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	9	PRO	3.7
1	E	289	ILE	3.5
1	A	277	HIS	3.5
1	A	290	GLY	3.4
1	E	277	HIS	3.2
1	A	286	ALA	3.1
1	H	77	GLU	3.0
1	C	172	ARG	3.0
1	E	172	ARG	3.0
1	A	171	ASP	2.9
1	H	172	ARG	2.8
1	A	173	ASP	2.8
1	B	172	ARG	2.8
1	H	171	ASP	2.8
1	A	287	GLY	2.8
1	A	172	ARG	2.7
1	E	285	ASP	2.7
1	C	12	GLU	2.7
1	D	12	GLU	2.6
1	D	77	GLU	2.6
1	H	74	ILE	2.6
1	C	522	PRO	2.6
1	H	8	LYS	2.5
1	D	9	PRO	2.5
1	E	287	GLY	2.5
1	E	290	GLY	2.5
1	A	480	ASP	2.5
1	D	80	ARG	2.4
1	H	173	ASP	2.4
1	D	54	ARG	2.4
1	E	294	GLU	2.3
1	H	174	GLY	2.3
1	H	187	ARG	2.3
1	H	522	PRO	2.3
1	H	75	SER	2.3
1	A	292	GLU	2.2
1	B	522	PRO	2.2
1	C	8	LYS	2.2
1	D	74	ILE	2.1
1	B	177	LEU	2.1
1	D	172	ARG	2.1
1	H	199	LEU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	294	GLU	2.1
1	B	171	ASP	2.1
1	C	171	ASP	2.1
1	B	77	GLU	2.1
1	B	199	LEU	2.1
1	E	284	LEU	2.1
1	D	171	ASP	2.1
1	D	173	ASP	2.1
1	G	172	ARG	2.1
1	A	288	ASP	2.1
1	A	187	ARG	2.1
1	A	291	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	MDO	A	149	13/14	0.92	0.08	11,15,18,19	0
1	MDO	F	149	13/14	0.93	0.08	9,14,18,19	0
1	MDO	H	149	13/14	0.93	0.09	13,16,20,21	0
1	MDO	D	149	13/14	0.94	0.07	14,16,18,20	0
1	MDO	G	149	13/14	0.94	0.07	8,12,14,17	0
1	MDO	E	149	13/14	0.94	0.07	9,12,16,19	0
1	MDO	B	149	13/14	0.95	0.07	11,14,17,18	0
1	MDO	C	149	13/14	0.96	0.06	9,10,14,15	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	TCA	B	701	11/11	0.88	0.10	22,23,29,29	0
2	TCA	D	701	11/11	0.88	0.12	24,30,31,31	0
2	TCA	H	701	11/11	0.88	0.13	34,35,38,39	0
2	TCA	E	701	11/11	0.90	0.09	21,23,24,25	0
2	TCA	C	701	11/11	0.91	0.08	20,21,23,23	0
2	TCA	A	701	11/11	0.91	0.09	22,23,26,26	0
2	TCA	G	701	11/11	0.92	0.09	19,22,24,25	0
2	TCA	F	701	11/11	0.93	0.07	21,24,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.