Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 03:19 PM EDT

PDB ID	:	1I7O
Title	:	CRYSTAL STRUCTURE OF HPCE
Authors	:	Tame, J.R.H.; Namba, K.; Dodson, E.J.; Roper, D.I.
Deposited on	:	2001-03-10
Resolution	:	1.70 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 (i) 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 (1)) were used in the production of this report:

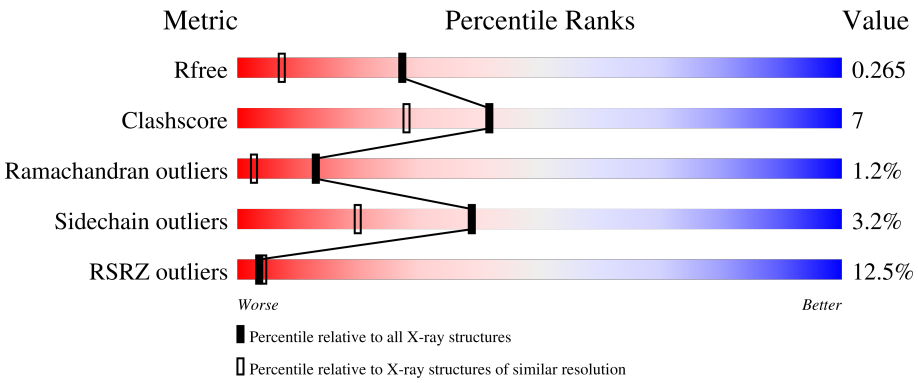
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 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 <=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	429	8% 84% 12% • •
1	B	429	10% 82% 14% • • •
1	C	429	10% 81% 15% • •
1	D	429	21% 77% 18% • • •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 13619 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 4-HYDROXYPHENYLACETATE DEGRADATION BIFUNCTIONAL ISOMERASE/DECARBOXYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	421	3237	2053	554	619	11	11	1	0
1	B	421	3237	2053	554	619	11	21	1	0
1	C	421	3237	2053	554	619	11	15	1	0
1	D	421	3236	2053	554	618	11	16	1	0

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
2	A	1	1	1	0	0
2	B	1	1	1	0	0
2	C	1	1	1	0	0
2	D	1	1	1	0	0

- Molecule 3 is water.

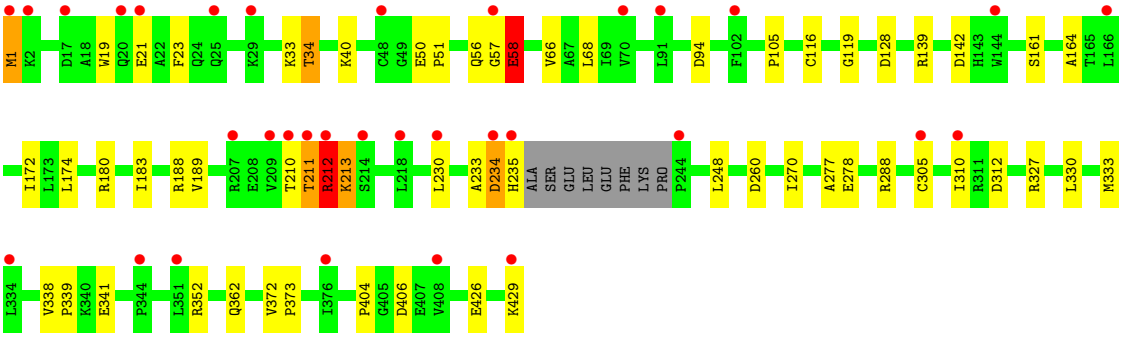
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	214	214	214	0	0
3	B	174	174	174	0	0
3	C	165	165	165	0	0
3	D	115	115	115	0	0

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.

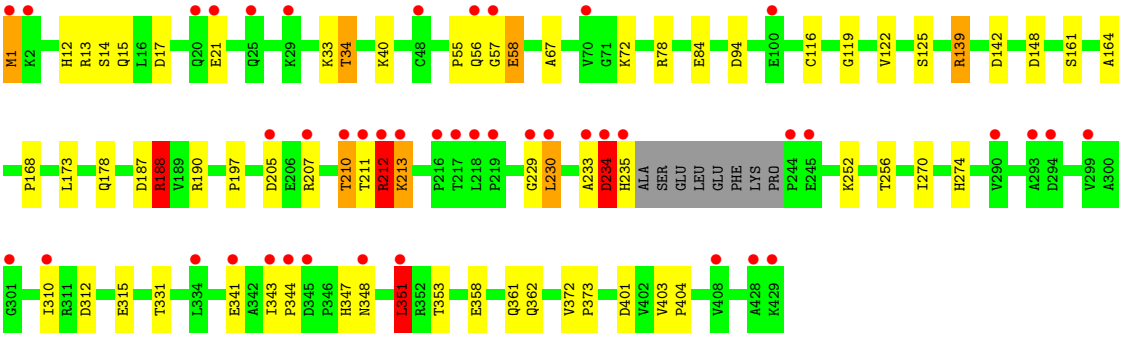
• Molecule 1: 4-HYDROXYPHENYLACETATE DEGRADATION BIFUNCTIONAL ISOMERASE/DECARBOXYLASE

Chain A:



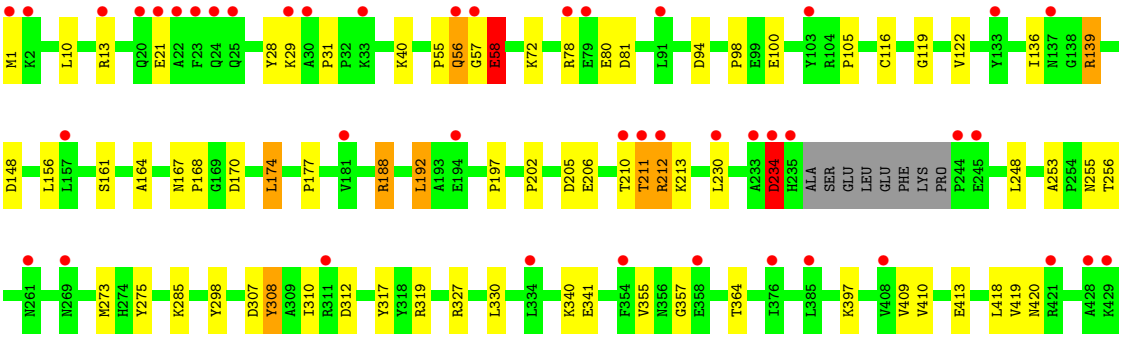
• Molecule 1: 4-HYDROXYPHENYLACETATE DEGRADATION BIFUNCTIONAL ISOMERASE/DECARBOXYLASE

Chain B:



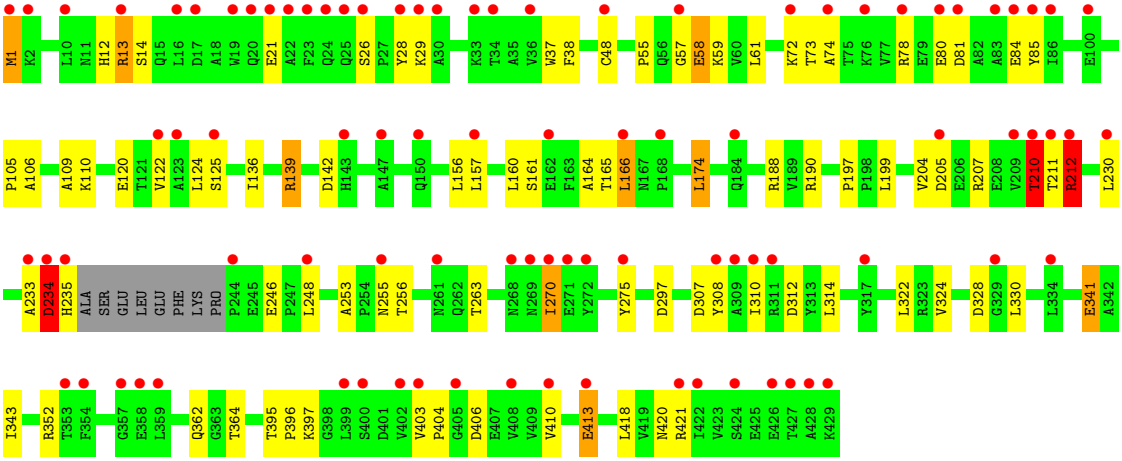
• Molecule 1: 4-HYDROXYPHENYLACETATE DEGRADATION BIFUNCTIONAL ISOMERASE/DECARBOXYLASE

Chain C:



• Molecule 1: 4-HYDROXYPHENYLACETATE DEGRADATION BIFUNCTIONAL ISOMERASE/DECARBOXYLASE

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	126.08Å 138.20Å 103.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 1.70 14.99 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.8 (15.00-1.70) 98.8 (14.99-1.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.64 (at 1.70Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.251 , 0.278 0.234 , 0.265	Depositor DCC
R_{free} test set	9927 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	30.4	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 53.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13619	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 26.47 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.6190e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: CA

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	0.98	3/3316 (0.1%)	1.01	9/4525 (0.2%)
1	B	0.94	5/3316 (0.2%)	0.99	16/4525 (0.4%)
1	C	0.91	3/3316 (0.1%)	1.02	13/4525 (0.3%)
1	D	0.86	2/3315 (0.1%)	1.02	13/4523 (0.3%)
All	All	0.92	13/13263 (0.1%)	1.01	51/18098 (0.3%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	139	ARG	CG-CD	17.47	1.95	1.51
1	A	212	ARG	CG-CD	-17.25	1.08	1.51
1	C	212	ARG	CG-CD	16.94	1.94	1.51
1	D	139	ARG	CB-CG	-16.49	1.08	1.52
1	C	188	ARG	CG-CD	-11.17	1.24	1.51
1	B	188	ARG	CG-CD	7.75	1.71	1.51
1	D	413	GLU	CD-OE2	7.35	1.33	1.25
1	A	333	MET	CG-SD	-6.35	1.64	1.81
1	C	308	TYR	CB-CG	5.82	1.60	1.51
1	A	277	ALA	CA-CB	5.42	1.63	1.52
1	B	358	GLU	CD-OE1	5.35	1.31	1.25
1	B	212	ARG	CG-CD	5.29	1.65	1.51
1	B	190	ARG	CG-CD	5.05	1.64	1.51

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	212	ARG	CG-CD-NE	-11.84	86.94	111.80
1	C	205	ASP	CB-CG-OD2	10.66	127.90	118.30
1	C	188	ARG	CB-CG-CD	10.29	138.36	111.60
1	C	212	ARG	CB-CG-CD	-9.09	87.97	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	139	ARG	CA-CB-CG	8.60	132.33	113.40
1	B	188	ARG	CG-CD-NE	8.43	129.50	111.80
1	D	307	ASP	CB-CG-OD2	7.98	125.48	118.30
1	D	234	ASP	CB-CG-OD2	7.65	125.18	118.30
1	A	212	ARG	CB-CG-CD	7.62	131.40	111.60
1	D	160	LEU	CB-CG-CD2	-7.59	98.09	111.00
1	A	260	ASP	CB-CG-OD2	7.39	124.95	118.30
1	A	406	ASP	CB-CG-OD1	6.96	124.56	118.30
1	B	33	LYS	CB-CG-CD	6.71	129.06	111.60
1	A	139	ARG	NE-CZ-NH1	-6.69	116.95	120.30
1	B	139	ARG	CB-CG-CD	-6.65	94.31	111.60
1	C	188	ARG	CG-CD-NE	6.63	125.72	111.80
1	C	148	ASP	CB-CG-OD2	6.56	124.21	118.30
1	D	212	ARG	CG-CD-NE	-6.53	98.09	111.80
1	D	190	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	B	142	ASP	CB-CG-OD2	6.37	124.03	118.30
1	B	212	ARG	CG-CD-NE	-6.33	98.51	111.80
1	C	307	ASP	CB-CG-OD2	6.19	123.87	118.30
1	D	190	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	D	142	ASP	CB-CG-OD2	5.97	123.67	118.30
1	C	234	ASP	CB-CG-OD2	5.93	123.64	118.30
1	C	81	ASP	CB-CG-OD2	5.84	123.56	118.30
1	B	148	ASP	CB-CG-OD2	5.78	123.50	118.30
1	A	288	ARG	NE-CZ-NH1	-5.63	117.49	120.30
1	C	94	ASP	CB-CG-OD2	5.59	123.33	118.30
1	B	13	ARG	NE-CZ-NH1	-5.57	117.52	120.30
1	C	139	ARG	CB-CG-CD	-5.55	97.18	111.60
1	A	234	ASP	CB-CG-OD2	5.43	123.19	118.30
1	B	94	ASP	CB-CG-OD2	5.43	123.19	118.30
1	B	351	LEU	CA-CB-CG	5.38	127.68	115.30
1	A	142	ASP	CB-CG-OD2	5.34	123.11	118.30
1	C	170	ASP	CB-CG-OD2	5.33	123.10	118.30
1	D	297	ASP	CB-CG-OD2	5.26	123.04	118.30
1	B	234	ASP	CB-CG-OD2	5.26	123.03	118.30
1	C	174	LEU	CB-CG-CD1	-5.24	102.09	111.00
1	D	81	ASP	CB-CG-OD2	5.24	123.02	118.30
1	D	330	LEU	CB-CG-CD2	-5.21	102.14	111.00
1	B	210	THR	N-CA-C	5.18	124.98	111.00
1	A	94	ASP	CB-CG-OD2	5.15	122.94	118.30
1	D	174	LEU	CA-CB-CG	-5.14	103.48	115.30
1	D	210	THR	N-CA-C	5.14	124.87	111.00
1	B	187	ASP	CB-CG-OD2	5.10	122.89	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	128	ASP	CB-CG-OD1	5.09	122.88	118.30
1	B	33	LYS	CD-CE-NZ	5.06	123.35	111.70
1	B	212	ARG	CB-CG-CD	-5.05	98.48	111.60
1	B	17	ASP	CB-CG-OD2	5.04	122.83	118.30
1	B	401	ASP	CB-CG-OD2	5.03	122.83	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3237	0	3193	32	3
1	B	3237	0	3195	41	16
1	C	3237	0	3195	43	5
1	D	3236	0	3193	63	22
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	214	0	0	3	0
3	B	174	0	0	1	0
3	C	165	0	0	3	0
3	D	115	0	0	2	0
All	All	13619	0	12776	178	23

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 7.

All (178) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:MET:CE	1:B:1:MET:SD	2.02	1.45
1:B:57:GLY:HA3	1:B:58:GLU:HB2	1.25	1.18
1:D:205:ASP:OD2	1:D:207:ARG:NH2	1.89	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:GLY:HA3	1:C:58:GLU:HB2	1.10	1.05
1:A:57:GLY:HA3	1:A:58:GLU:HB2	1.38	1.03
1:D:57:GLY:HA3	1:D:58:GLU:HB2	1.38	1.00
1:C:57:GLY:CA	1:C:58:GLU:HB2	1.92	0.99
1:B:57:GLY:CA	1:B:58:GLU:HB2	1.92	0.98
1:D:1:MET:N	1:D:1:MET:HE3	1.80	0.96
1:C:308:TYR:OH	1:C:420:ASN:ND2	2.05	0.89
1:D:157:LEU:CD1	1:D:166:LEU:HD13	2.04	0.88
1:A:57:GLY:CA	1:A:58:GLU:HB2	2.05	0.85
1:D:57:GLY:CA	1:D:58:GLU:HB2	2.08	0.82
1:D:74:ALA:HB3	1:D:166:LEU:HB2	1.59	0.82
1:B:122:VAL:HG21	1:B:197:PRO:HD3	1.63	0.80
1:D:13:ARG:HH11	1:D:13:ARG:HG3	1.46	0.78
1:A:56:GLN:HG3	1:A:57:GLY:H	1.47	0.78
1:A:56:GLN:HG3	1:A:57:GLY:N	1.99	0.77
1:D:1:MET:HE3	1:D:1:MET:H2	1.49	0.77
1:A:352:ARG:NE	1:A:362:GLN:OE1	2.11	0.77
1:B:233:ALA:O	1:B:235:HIS:N	2.17	0.77
1:D:13:ARG:HH11	1:D:13:ARG:CG	1.98	0.77
1:B:211:THR:O	1:B:212:ARG:HB2	1.84	0.76
1:C:122:VAL:HG21	1:C:197:PRO:HD3	1.67	0.75
1:B:347:HIS:NE2	1:B:372:VAL:HG23	2.01	0.75
1:D:1:MET:N	1:D:1:MET:CE	2.50	0.74
1:B:372:VAL:HB	1:B:373:PRO:HD3	1.68	0.74
1:D:157:LEU:HD11	1:D:166:LEU:HD13	1.68	0.74
1:C:56:GLN:HE21	1:C:57:GLY:H	1.33	0.73
1:B:252:LYS:NZ	1:B:331:THR:OG1	2.14	0.73
1:A:211:THR:O	1:A:212:ARG:HB2	1.90	0.72
1:B:122:VAL:HG21	1:B:197:PRO:CD	2.21	0.70
1:C:410:VAL:CG2	1:C:418:LEU:HB3	2.21	0.70
1:D:210:THR:HB	1:D:211:THR:HG23	1.74	0.70
1:D:410:VAL:HG23	1:D:418:LEU:HB3	1.74	0.69
1:D:13:ARG:HG3	1:D:13:ARG:NH1	2.04	0.68
1:D:72:LYS:HG3	1:D:85:TYR:CD2	2.29	0.68
1:C:13:ARG:HG2	1:C:13:ARG:HH11	1.59	0.67
1:D:1:MET:HE3	1:D:1:MET:H1	1.57	0.67
1:A:278:GLU:HB2	1:A:305:CYS:SG	2.35	0.67
1:B:205:ASP:OD2	1:B:207:ARG:NH2	2.24	0.65
1:C:410:VAL:HG23	1:C:418:LEU:HB3	1.80	0.64
1:C:57:GLY:HA3	1:C:58:GLU:CB	2.05	0.64
1:D:1:MET:H2	1:D:1:MET:CE	2.10	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:156:LEU:HD12	1:D:174:LEU:HD22	1.80	0.62
1:C:234:ASP:HB3	1:C:397:LYS:CG	2.30	0.61
1:A:183:ILE:HG21	1:A:189:VAL:HG21	1.83	0.61
1:D:308:TYR:OH	1:D:420:ASN:ND2	2.33	0.61
1:C:161:SER:HA	1:C:164:ALA:O	2.00	0.60
1:C:1:MET:HE3	1:C:119:GLY:O	2.01	0.59
1:C:56:GLN:NE2	1:C:57:GLY:H	2.00	0.59
1:D:1:MET:HE2	1:D:1:MET:HA	1.83	0.59
1:D:234:ASP:HB3	1:D:397:LYS:CG	2.34	0.58
1:A:1:MET:HE3	1:A:119:GLY:O	2.05	0.57
1:D:1:MET:CE	1:D:1:MET:CA	2.83	0.57
1:D:12:HIS:HD2	1:D:14:SER:OG	1.87	0.57
1:D:403:VAL:O	1:D:406:ASP:HB2	2.04	0.57
1:A:34:THR:HG21	3:A:1187:HOH:O	2.04	0.56
1:D:28:TYR:O	1:D:29:LYS:HB3	2.06	0.56
1:A:66:VAL:HG13	1:A:174:LEU:HD12	1.87	0.56
1:B:270:ILE:HD13	1:B:310:ILE:HG23	1.87	0.56
1:D:72:LYS:HG3	1:D:85:TYR:HD2	1.68	0.56
1:C:40:LYS:HE3	1:C:116:CYS:HB2	1.87	0.55
1:C:413:GLU:HG3	3:C:1123:HOH:O	2.06	0.55
1:D:106:ALA:HB1	1:D:109:ALA:HB3	1.89	0.55
1:A:56:GLN:HE21	1:A:57:GLY:H	1.53	0.55
1:D:122:VAL:HG12	1:D:124:LEU:HG	1.89	0.54
1:B:403:VAL:HB	1:B:404:PRO:HD2	1.88	0.54
1:D:253:ALA:O	1:D:256:THR:HG22	2.08	0.54
1:D:12:HIS:CD2	1:D:14:SER:OG	2.61	0.53
1:D:37:TRP:HB2	1:D:322:LEU:HG	1.90	0.53
1:B:67:ALA:HB2	1:B:173:LEU:CD2	2.39	0.53
1:B:57:GLY:CA	1:B:58:GLU:CB	2.76	0.53
1:D:211:THR:O	1:D:212:ARG:HB2	2.08	0.53
1:D:343:ILE:HG22	1:D:343:ILE:O	2.09	0.53
1:D:156:LEU:CD1	1:D:174:LEU:HD22	2.39	0.52
1:B:56:GLN:HE21	1:B:57:GLY:H	1.57	0.52
1:B:274:HIS:HE1	3:B:1116:HOH:O	1.92	0.52
1:A:56:GLN:CG	1:A:57:GLY:H	2.20	0.52
1:D:165:THR:O	1:D:255:ASN:ND2	2.35	0.52
1:B:67:ALA:HB2	1:B:173:LEU:HD23	1.92	0.51
1:C:327:ARG:HB2	3:C:1128:HOH:O	2.09	0.51
1:B:55:PRO:O	1:B:58:GLU:HB3	2.11	0.51
1:C:211:THR:O	1:C:212:ARG:HB2	2.11	0.51
1:B:161:SER:HA	1:B:164:ALA:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:341:GLU:H	1:D:341:GLU:CD	2.15	0.50
1:A:270:ILE:HD13	1:A:310:ILE:HG23	1.92	0.50
1:B:122:VAL:CG2	1:B:197:PRO:CD	2.88	0.50
1:B:15:GLN:HG3	1:B:178:GLN:OE1	2.11	0.49
1:C:409:VAL:HG22	1:C:419:VAL:HG22	1.93	0.49
1:A:19:TRP:CE3	1:A:23:PHE:CE1	3.00	0.49
1:B:1:MET:HE3	1:B:119:GLY:O	2.12	0.49
1:A:56:GLN:CG	1:A:57:GLY:N	2.74	0.49
1:B:56:GLN:NE2	1:B:57:GLY:H	2.11	0.49
1:C:28:TYR:O	1:C:29:LYS:HB3	2.13	0.49
1:D:270:ILE:HD13	1:D:310:ILE:HG23	1.94	0.49
1:A:105:PRO:HD2	1:A:248:LEU:HD21	1.94	0.48
1:C:72:LYS:HA	1:C:168:PRO:HG3	1.94	0.48
1:A:330:LEU:CD1	3:A:1036:HOH:O	2.61	0.48
1:C:355:VAL:C	1:C:357:GLY:N	2.65	0.48
1:A:330:LEU:HD11	3:A:1036:HOH:O	2.13	0.48
1:B:12:HIS:HD2	1:B:14:SER:H	1.62	0.48
1:A:40:LYS:HE3	1:A:116:CYS:HB2	1.95	0.48
1:B:72:LYS:HA	1:B:168:PRO:HG3	1.96	0.48
1:C:13:ARG:HG2	1:C:13:ARG:NH1	2.28	0.47
1:D:275:TYR:HA	1:D:308:TYR:CD1	2.49	0.47
1:A:233:ALA:O	1:A:235:HIS:N	2.47	0.47
1:C:327:ARG:HD3	1:C:330:LEU:HD22	1.97	0.47
1:D:72:LYS:HE3	1:D:84:GLU:HG3	1.97	0.47
1:D:263:THR:HA	1:D:421:ARG:O	2.15	0.47
1:D:410:VAL:CG2	1:D:418:LEU:HD23	2.45	0.47
1:B:213:LYS:HE3	1:B:213:LYS:HB2	1.43	0.47
1:B:229:GLY:O	1:B:230:LEU:C	2.52	0.47
1:D:157:LEU:CD1	1:D:166:LEU:CD1	2.87	0.47
1:B:351:LEU:O	1:B:362:GLN:HA	2.15	0.47
1:C:98:PRO:HB2	1:C:100:GLU:HG3	1.96	0.47
1:C:192:LEU:HD12	1:C:192:LEU:N	2.30	0.47
1:A:372:VAL:HB	1:A:373:PRO:HD3	1.97	0.46
1:D:1:MET:HE2	1:D:1:MET:CA	2.44	0.46
1:C:105:PRO:HD3	1:C:319:ARG:O	2.16	0.46
1:C:275:TYR:C	1:C:275:TYR:CD1	2.87	0.46
1:D:410:VAL:HG21	1:D:418:LEU:HD23	1.98	0.46
1:B:34:THR:HB	1:B:315:GLU:OE2	2.16	0.46
1:C:285:LYS:HD2	1:C:298:TYR:CE2	2.51	0.46
1:A:161:SER:HA	1:A:164:ALA:O	2.15	0.46
1:D:248:LEU:C	1:D:248:LEU:HD13	2.36	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:229:GLY:O	1:B:230:LEU:O	2.35	0.45
1:C:31:PRO:HA	1:C:317:TYR:OH	2.17	0.45
1:C:253:ALA:O	1:C:256:THR:HG22	2.16	0.45
1:D:161:SER:HA	1:D:164:ALA:O	2.16	0.45
1:C:210:THR:O	1:C:212:ARG:N	2.49	0.45
1:A:180:ARG:HH11	1:A:180:ARG:HD3	1.63	0.45
1:B:1:MET:CE	1:B:1:MET:CG	2.91	0.45
1:B:403:VAL:HB	1:B:404:PRO:CD	2.46	0.44
1:C:55:PRO:HA	1:C:206:GLU:CD	2.37	0.44
1:C:57:GLY:CA	1:C:58:GLU:CB	2.77	0.44
1:A:338:VAL:HA	1:A:339:PRO:HD3	1.88	0.44
1:A:426:GLU:O	1:A:429:LYS:HG2	2.18	0.44
1:B:256:THR:HG23	1:B:331:THR:HB	1.99	0.44
1:C:156:LEU:HD12	1:C:174:LEU:CD2	2.48	0.44
1:D:48[B]:CYS:HB2	1:D:199:LEU:HD12	1.99	0.44
1:C:167:ASN:HD21	1:C:255:ASN:HD21	1.65	0.44
1:B:353:THR:HB	1:B:361:GLN:HB3	1.98	0.44
1:C:410:VAL:HG22	1:C:418:LEU:HB3	1.99	0.44
1:D:72:LYS:O	1:D:73:THR:C	2.56	0.44
1:D:105:PRO:HD2	1:D:248:LEU:HD21	1.99	0.43
1:C:10:LEU:HD23	1:C:10:LEU:HA	1.81	0.43
1:D:233:ALA:O	1:D:235:HIS:N	2.52	0.43
1:D:120:GLU:HB3	1:D:197:PRO:HG2	2.01	0.42
1:B:40:LYS:HE3	1:B:116:CYS:HB2	2.00	0.42
1:D:12:HIS:HE1	3:D:1070:HOH:O	2.02	0.42
1:D:55:PRO:O	1:D:58:GLU:HB3	2.19	0.42
1:D:78:ARG:NH2	1:D:80:GLU:OE2	2.49	0.42
1:D:314:LEU:HD23	1:D:324:VAL:HG21	2.01	0.42
1:B:12:HIS:CD2	1:B:14:SER:H	2.38	0.42
1:C:156:LEU:HD12	1:C:174:LEU:HD22	2.00	0.42
1:D:204:VAL:HA	3:D:1106:HOH:O	2.20	0.42
1:D:72:LYS:HG2	1:D:85:TYR:HA	2.02	0.42
1:A:211:THR:O	1:A:212:ARG:CB	2.61	0.42
1:D:403:VAL:HB	1:D:404:PRO:HD2	2.02	0.42
1:B:343:ILE:HA	1:B:344:PRO:HD2	1.90	0.41
1:C:177:PRO:HD2	3:C:1017:HOH:O	2.19	0.41
1:D:59:LYS:HE2	1:D:61:LEU:HD21	2.01	0.41
1:A:50:GLU:HA	1:A:51:PRO:HD3	1.94	0.41
1:A:68:LEU:HD21	1:A:172:ILE:HD12	2.02	0.41
1:B:57:GLY:N	1:B:58:GLU:HB2	2.33	0.41
1:B:40:LYS:CE	1:B:116:CYS:HB2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:ARG:NH2	1:C:340:LYS:HD2	2.36	0.41
1:D:38:PHE:CE2	1:D:110:LYS:HD3	2.56	0.41
1:A:327:ARG:HD3	1:A:330:LEU:HD22	2.03	0.41
1:C:78:ARG:NH2	1:C:80:GLU:OE2	2.54	0.41
1:C:273:MET:HG3	1:C:310:ILE:HD13	2.02	0.40
1:D:174:LEU:HA	1:D:174:LEU:HD23	1.60	0.40
1:A:213:LYS:HB2	1:A:213:LYS:HE3	1.67	0.40
1:D:395:THR:OG1	1:D:396:PRO:HD2	2.20	0.40
1:C:122:VAL:HG21	1:C:197:PRO:CD	2.45	0.40
1:A:19:TRP:HE3	1:A:23:PHE:CE1	2.40	0.40
1:D:164:ALA:HA	1:D:328:ASP:OD1	2.21	0.40

All (23) 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:139:ARG:NH1	1:D:13:ARG:CZ[2_554]	0.75	1.45
1:B:139:ARG:NH2	1:D:13:ARG:NH2[2_554]	0.75	1.45
1:B:139:ARG:CZ	1:D:13:ARG:CZ[2_554]	0.83	1.37
1:B:139:ARG:NH1	1:D:13:ARG:NE[2_554]	1.09	1.11
1:B:139:ARG:CZ	1:D:13:ARG:NH2[2_554]	1.11	1.09
1:B:139:ARG:NH1	1:D:13:ARG:NH1[2_554]	1.24	0.96
1:C:139:ARG:NH1	1:D:136:ILE:O[4_556]	1.42	0.78
1:B:139:ARG:CZ	1:D:13:ARG:NE[2_554]	1.61	0.59
1:B:139:ARG:NH2	1:D:13:ARG:CZ[2_554]	1.61	0.59
1:B:139:ARG:NH1	1:D:13:ARG:CD[2_554]	1.86	0.34
1:B:139:ARG:CZ	1:D:13:ARG:NH1[2_554]	1.88	0.32
1:B:188:ARG:NH2	1:C:202:PRO:CB[4_556]	1.90	0.30
1:B:139:ARG:NE	1:D:13:ARG:NH2[2_554]	2.04	0.16
1:A:33:LYS:CD	1:D:352:ARG:NH2[4_546]	2.05	0.15
1:B:139:ARG:NE	1:D:13:ARG:NE[2_554]	2.05	0.15
1:B:139:ARG:NH1	1:D:13:ARG:NH2[2_554]	2.07	0.13
1:B:139:ARG:NE	1:D:13:ARG:CZ[2_554]	2.07	0.13
1:C:136:ILE:CB	1:D:139:ARG:NH2[4_556]	2.07	0.13
1:A:33:LYS:CE	1:D:362:GLN:OE1[4_546]	2.10	0.10
1:C:139:ARG:NH2	1:D:136:ILE:CG2[4_556]	2.10	0.10
1:B:139:ARG:NH2	1:D:13:ARG:NH1[2_554]	2.16	0.04
1:A:33:LYS:NZ	1:D:362:GLN:OE1[4_546]	2.19	0.01
1:C:136:ILE:CG2	1:D:139:ARG:NH2[4_556]	2.19	0.01

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	418/429 (97%)	404 (97%)	9 (2%)	5 (1%)	13 3
1	B	418/429 (97%)	402 (96%)	11 (3%)	5 (1%)	13 3
1	C	418/429 (97%)	400 (96%)	14 (3%)	4 (1%)	15 4
1	D	418/429 (97%)	398 (95%)	14 (3%)	6 (1%)	11 2
All	All	1672/1716 (97%)	1604 (96%)	48 (3%)	20 (1%)	13 3

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	58	GLU
1	A	210	THR
1	A	230	LEU
1	A	234	ASP
1	B	58	GLU
1	B	210	THR
1	B	230	LEU
1	B	234	ASP
1	C	58	GLU
1	C	211	THR
1	D	58	GLU
1	D	210	THR
1	D	234	ASP
1	D	230	LEU
1	C	234	ASP
1	D	413	GLU
1	D	212	ARG
1	A	212	ARG
1	B	212	ARG
1	C	230	LEU

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	348/360 (97%)	338 (97%)	10 (3%)	42	23
1	B	348/360 (97%)	336 (97%)	12 (3%)	37	18
1	C	348/360 (97%)	337 (97%)	11 (3%)	39	20
1	D	348/360 (97%)	336 (97%)	12 (3%)	37	18
All	All	1392/1440 (97%)	1347 (97%)	45 (3%)	39	20

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	21	GLU
1	A	34	THR
1	A	58	GLU
1	A	188	ARG
1	A	211	THR
1	A	213	LYS
1	A	312	ASP
1	A	341	GLU
1	A	404	PRO
1	B	1	MET
1	B	21	GLU
1	B	34	THR
1	B	84	GLU
1	B	125	SER
1	B	188	ARG
1	B	213	LYS
1	B	234	ASP
1	B	312	ASP
1	B	341	GLU
1	B	348	ASN
1	B	351	LEU
1	C	21	GLU
1	C	56	GLN

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Mol	Chain	Res	Type
1	C	58	GLU
1	C	188	ARG
1	C	192	LEU
1	C	213	LYS
1	C	234	ASP
1	C	248	LEU
1	C	312	ASP
1	C	341	GLU
1	C	364	THR
1	D	1	MET
1	D	13	ARG
1	D	21	GLU
1	D	26	SER
1	D	125	SER
1	D	166	LEU
1	D	188	ARG
1	D	246	GLU
1	D	270	ILE
1	D	312	ASP
1	D	341	GLU
1	D	364	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	56	GLN
1	A	129	ASN
1	A	150	GLN
1	A	201	ASN
1	A	268	ASN
1	A	274	HIS
1	A	286	GLN
1	A	348	ASN
1	A	386	ASN
1	A	420	ASN
1	B	12	HIS
1	B	15	GLN
1	B	25	GLN
1	B	56	GLN
1	B	268	ASN
1	B	274	HIS

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Mol	Chain	Res	Type
1	B	286	GLN
1	B	348	ASN
1	B	386	ASN
1	B	420	ASN
1	C	12	HIS
1	C	15	GLN
1	C	25	GLN
1	C	56	GLN
1	C	150	GLN
1	C	167	ASN
1	C	268	ASN
1	C	420	ASN
1	D	12	HIS
1	D	25	GLN
1	D	201	ASN
1	D	268	ASN
1	D	286	GLN
1	D	386	ASN
1	D	420	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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(Å^2)	Q<0.9
1	A	421/429 (98%)	0.54	33 (7%)	13	15	32, 39, 56, 72	5 (1%)
1	B	421/429 (98%)	0.64	44 (10%)	6	7	33, 42, 62, 79	7 (1%)
1	C	421/429 (98%)	0.69	44 (10%)	6	7	31, 43, 61, 78	5 (1%)
1	D	421/429 (98%)	1.25	90 (21%)	0	0	32, 47, 68, 83	5 (1%)
All	All	1684/1716 (98%)	0.78	211 (12%)	3	4	31, 43, 63, 83	22 (1%)

All (211) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	211	THR	11.4
1	B	334	LEU	11.0
1	A	334	LEU	10.1
1	A	210	THR	9.3
1	B	235	HIS	9.3
1	D	235	HIS	9.0
1	C	334	LEU	9.0
1	D	428	ALA	9.0
1	B	244	PRO	8.3
1	D	427	THR	8.1
1	A	235	HIS	8.1
1	B	211	THR	7.7
1	C	1	MET	7.7
1	D	334	LEU	7.5
1	B	1	MET	7.3
1	C	235	HIS	7.3
1	A	244	PRO	7.2
1	D	1	MET	7.2
1	D	230	LEU	6.9
1	D	74	ALA	6.8
1	C	2	LYS	6.7

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Mol	Chain	Res	Type	RSRZ
1	D	211	THR	6.7
1	A	230	LEU	6.5
1	B	230	LEU	6.3
1	D	210	THR	6.3
1	D	2	LYS	6.1
1	B	210	THR	6.0
1	D	123	ALA	5.9
1	D	30	ALA	5.7
1	D	19	TRP	5.7
1	D	429	LYS	5.5
1	D	33	LYS	5.5
1	D	272	TYR	5.4
1	A	1	MET	5.4
1	B	2	LYS	5.3
1	C	230	LEU	5.2
1	A	211	THR	5.1
1	D	24	GLN	5.1
1	C	29	LYS	5.0
1	A	2	LYS	4.8
1	A	57	GLY	4.8
1	C	24	GLN	4.6
1	D	29	LYS	4.6
1	D	426	GLU	4.6
1	D	408	VAL	4.6
1	C	20	GLN	4.5
1	D	78	ARG	4.5
1	D	269	ASN	4.5
1	C	30	ALA	4.5
1	D	125	SER	4.3
1	C	57	GLY	4.2
1	D	57	GLY	4.2
1	D	270	ILE	4.1
1	D	261	ASN	4.1
1	D	405	GLY	4.1
1	B	344	PRO	4.0
1	D	17	ASP	4.0
1	D	21	GLU	3.9
1	B	429	LYS	3.9
1	D	25	GLN	3.9
1	A	234	ASP	3.9
1	B	48[A]	CYS	3.8
1	B	290	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	216	PRO	3.8
1	A	305	CYS	3.7
1	C	25	GLN	3.7
1	C	429	LYS	3.7
1	A	212	ARG	3.7
1	B	293	ALA	3.6
1	A	209	VAL	3.6
1	D	413	GLU	3.6
1	C	210	THR	3.6
1	A	70	VAL	3.6
1	C	33	LYS	3.5
1	D	76	LYS	3.5
1	D	359	LEU	3.4
1	D	422	ILE	3.4
1	D	80	GLU	3.4
1	D	244	PRO	3.4
1	C	245	GLU	3.4
1	D	212	ARG	3.3
1	D	26	SER	3.3
1	D	20	GLN	3.3
1	C	269	ASN	3.3
1	B	56	GLN	3.2
1	D	150	GLN	3.2
1	B	57	GLY	3.2
1	D	81	ASP	3.1
1	A	29	LYS	3.1
1	C	78	ARG	3.1
1	C	233	ALA	3.1
1	B	348	ASN	3.1
1	D	205	ASP	3.1
1	B	245	GLU	3.1
1	D	157	LEU	3.1
1	A	310	ILE	3.0
1	D	209	VAL	3.0
1	B	212	ARG	3.0
1	D	13	ARG	3.0
1	D	410	VAL	3.0
1	B	213	LYS	3.0
1	D	311	ARG	3.0
1	C	234	ASP	2.9
1	B	234	ASP	2.9
1	A	91	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	217	THR	2.9
1	C	428	ALA	2.8
1	C	244	PRO	2.8
1	A	166	LEU	2.8
1	D	234	ASP	2.8
1	D	309	ALA	2.8
1	B	218	LEU	2.8
1	C	21	GLU	2.7
1	D	85	TYR	2.7
1	B	70	VAL	2.7
1	C	181	VAL	2.7
1	D	16	LEU	2.7
1	D	329	GLY	2.7
1	B	343	ILE	2.7
1	B	428	ALA	2.6
1	D	358	GLU	2.6
1	A	344	PRO	2.6
1	A	48[A]	CYS	2.6
1	D	357	GLY	2.6
1	D	308	TYR	2.6
1	D	22	ALA	2.6
1	A	214	SER	2.6
1	B	341	GLU	2.6
1	B	20	GLN	2.6
1	C	157	LEU	2.6
1	D	271	GLU	2.5
1	C	56	GLN	2.5
1	D	168	PRO	2.5
1	C	137	ASN	2.5
1	A	429	LYS	2.5
1	D	275	TYR	2.5
1	D	255	ASN	2.5
1	D	268	ASN	2.5
1	B	294	ASP	2.5
1	B	233	ALA	2.5
1	C	212	ARG	2.5
1	D	402	VAL	2.5
1	C	13	ARG	2.4
1	A	17	ASP	2.4
1	A	21	GLU	2.4
1	C	194	GLU	2.4
1	B	345	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	207	ARG	2.4
1	C	385	LEU	2.4
1	D	84	GLU	2.4
1	C	311	ARG	2.4
1	D	100	GLU	2.4
1	A	351	LEU	2.4
1	D	353	THR	2.4
1	C	79	GLU	2.4
1	D	36	VAL	2.3
1	D	143	HIS	2.4
1	D	403	VAL	2.3
1	B	351	LEU	2.3
1	D	166	LEU	2.3
1	D	310	ILE	2.3
1	B	229	GLY	2.3
1	B	299	VAL	2.3
1	D	399	LEU	2.3
1	B	25	GLN	2.3
1	D	10	LEU	2.3
1	D	400	SER	2.3
1	C	376	ILE	2.3
1	D	233	ALA	2.3
1	C	358	GLU	2.3
1	D	23	PHE	2.3
1	D	28	TYR	2.3
1	B	301	GLY	2.3
1	C	408	VAL	2.2
1	D	122	VAL	2.2
1	D	147	ALA	2.2
1	B	310	ILE	2.2
1	A	20	GLN	2.2
1	C	23	PHE	2.2
1	C	103	TYR	2.2
1	C	22	ALA	2.2
1	C	421	ARG	2.2
1	B	219	PRO	2.2
1	C	354	PHE	2.2
1	B	21	GLU	2.2
1	D	48[A]	CYS	2.2
1	A	376	ILE	2.2
1	D	72	LYS	2.2
1	A	207	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	421	ARG	2.1
1	D	424	SER	2.1
1	A	102	PHE	2.1
1	B	205	ASP	2.1
1	D	162	GLU	2.1
1	B	29	LYS	2.1
1	C	261	ASN	2.1
1	B	408	VAL	2.1
1	A	218	LEU	2.1
1	D	248	LEU	2.1
1	D	86	ILE	2.1
1	B	100	GLU	2.1
1	A	25	GLN	2.0
1	D	34	THR	2.0
1	D	184	GLN	2.0
1	D	83	ALA	2.0
1	D	317	TYR	2.0
1	A	408	VAL	2.0
1	D	354	PHE	2.0
1	C	133	TYR	2.0
1	C	91	LEU	2.0
1	A	144	TRP	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 monosaccharides 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(Å^2)	Q<0.9
2	CA	D	1004	1/1	0.88	0.07	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CA	C	1003	1/1	0.99	0.08	42,42,42,42	0
2	CA	B	1002	1/1	0.99	0.04	40,40,40,40	0
2	CA	A	1001	1/1	1.00	0.06	35,35,35,35	0

6.5 Other polymers (i)

There are no such residues in this entry.