



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 07:31 PM GMT

PDB ID : 4TRQ
Title : Crystal structure of Sac3/Thp1/Sem1
Authors : Hellerschmied, D.; Schneider, S.; Kohler, A.; Clausen, T.
Deposited on : 2014-06-17
Resolution : 3.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
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-20026982

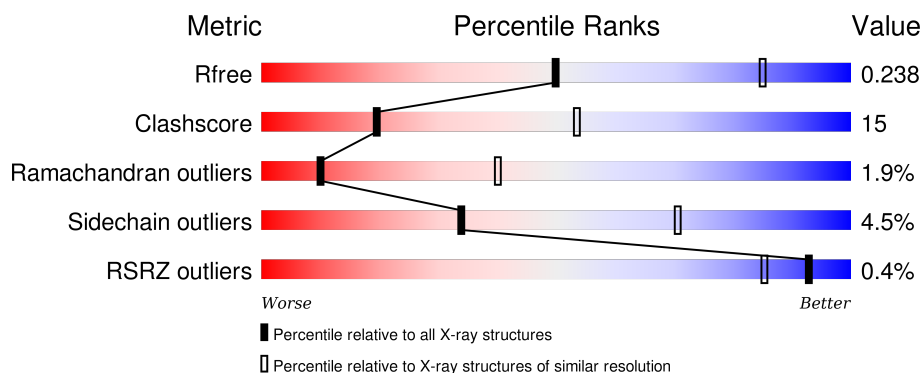
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	299	<div> <div>66%</div> <div>30%</div> <div>.</div> </div>
1	D	299	<div> <div>63%</div> <div>31%</div> <div>5%</div> </div>
2	B	286	<div> <div>77%</div> <div>21%</div> <div>.</div> </div>
2	E	286	<div> <div>69%</div> <div>29%</div> <div>.</div> </div>
3	C	60	<div> <div>55%</div> <div>17%</div> <div>10%</div> <div>18%</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	60	 A horizontal bar chart showing the quality of chain F. The bar is divided into four segments: red (2%), green (50%), yellow (27%), and grey (18%). The segments are labeled with their respective percentages: 2%, 50%, 27%, 5%, and 18%.

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10521 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 Nuclear mRNA export protein SAC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	299	Total	C	N	O	S	0	0	0
			2474	1582	426	453	13			
1	D	299	Total	C	N	O	S	0	0	0
			2474	1582	426	453	13			

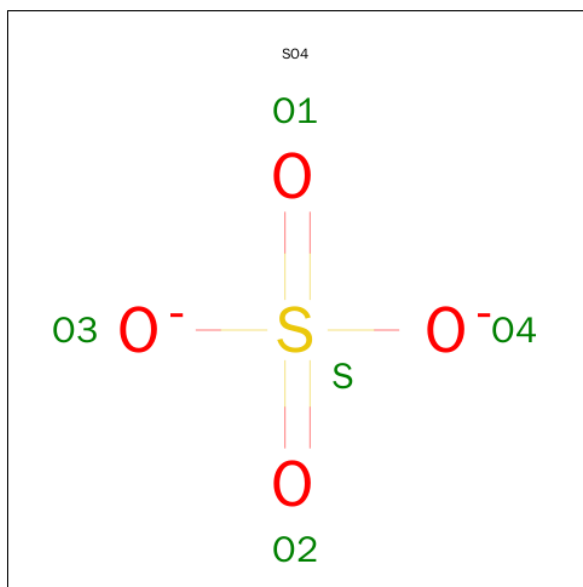
- Molecule 2 is a protein called Nuclear mRNA export protein THP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	286	Total	C	N	O	S	0	0	0
			2359	1533	410	406	10			
2	E	286	Total	C	N	O	S	0	0	0
			2359	1533	410	406	10			

- Molecule 3 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	49	Total	C	N	O	0	0	0
			425	260	65	100			
3	F	49	Total	C	N	O	0	0	0
			425	260	65	100			

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).

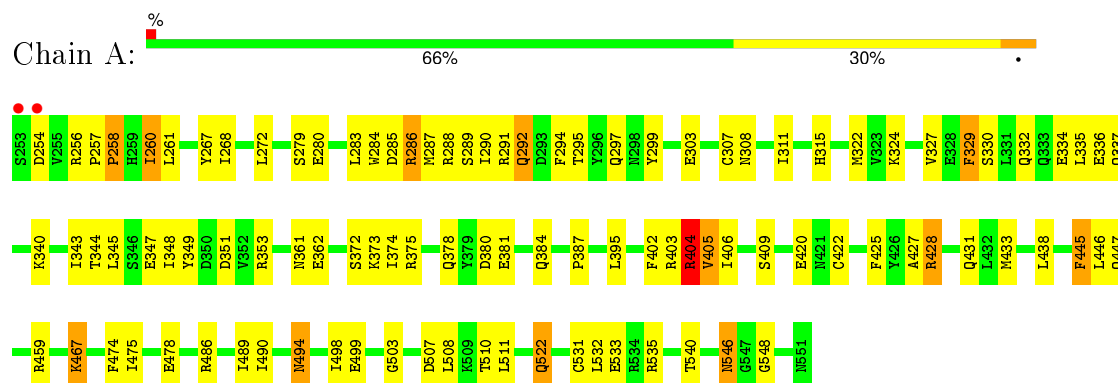


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		

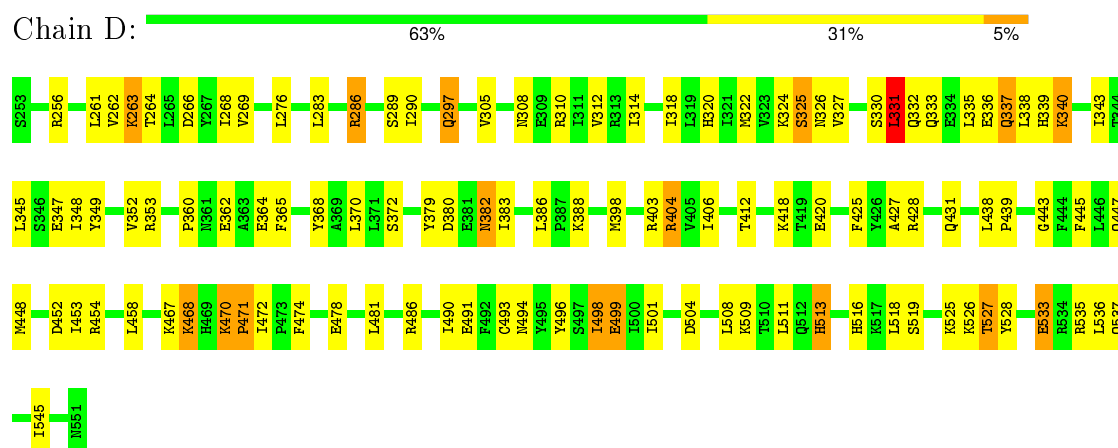
3 Residue-property plots

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.

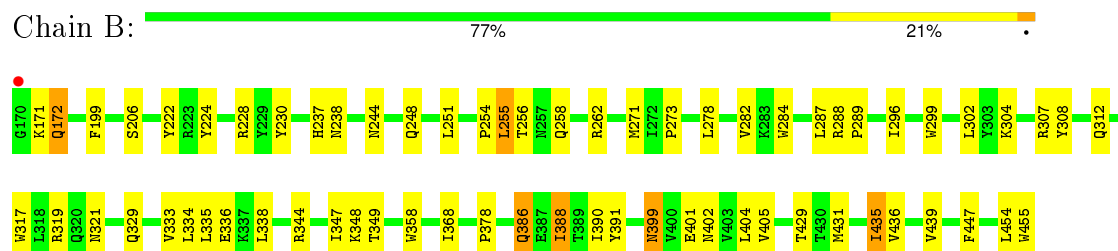
• Molecule 1: Nuclear mRNA export protein SAC3



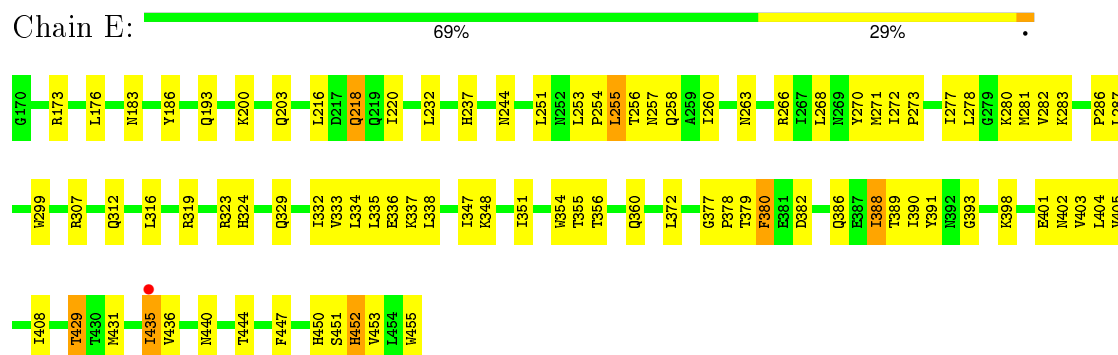
• Molecule 1: Nuclear mRNA export protein SAC3



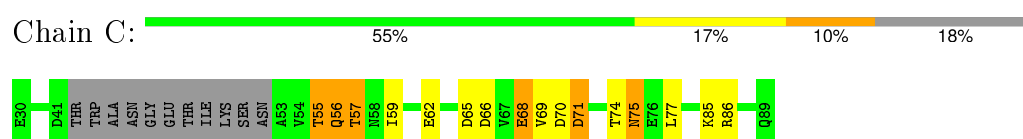
• Molecule 2: Nuclear mRNA export protein THP1



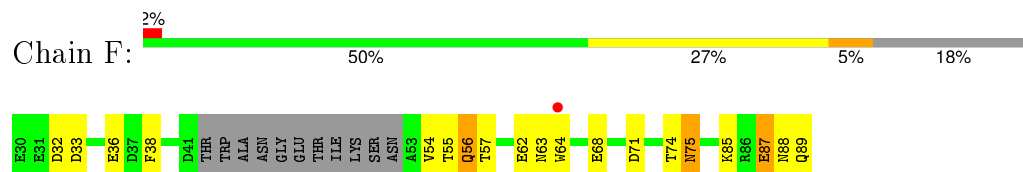
- Molecule 2: Nuclear mRNA export protein THP1



- Molecule 3: 26S proteasome complex subunit SEM1



- Molecule 3: 26S proteasome complex subunit SEM1



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	125.74Å 125.74Å 268.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.61 – 3.10 47.61 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.6 (47.61-3.10) 98.6 (47.61-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 3.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.194 , 0.238 0.194 , 0.238	Depositor DCC
R_{free} test set	1976 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	75.9	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 55.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 39371 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10521	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.39	0/2528	0.66	1/3415 (0.0%)
1	D	0.37	0/2528	0.63	1/3415 (0.0%)
2	B	0.40	0/2416	0.60	0/3282
2	E	0.37	0/2416	0.63	1/3282 (0.0%)
3	C	0.41	0/432	0.71	0/584
3	F	0.39	0/432	0.67	0/584
All	All	0.38	0/10752	0.63	3/14562 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	331	LEU	CA-CB-CG	6.46	130.17	115.30
1	A	404	ARG	CG-CD-NE	6.30	125.03	111.80
2	E	255	LEU	CA-CB-CG	5.60	128.18	115.30

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	2474	0	2473	97	0
1	D	2474	0	2473	95	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2359	0	2428	50	0
2	E	2359	0	2428	75	0
3	C	425	0	355	12	1
3	F	425	0	355	18	1
4	A	5	0	0	0	0
All	All	10521	0	10512	316	1

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 15.

All (316) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:513:HIS:HD2	1:D:518:LEU:HD22	1.26	1.00
1:A:490:ILE:O	1:A:494:ASN:ND2	2.02	0.92
1:D:388:LYS:HD3	2:E:323:ARG:HD2	1.55	0.87
1:D:513:HIS:CD2	1:D:518:LEU:HD22	2.12	0.84
1:D:398:MET:HE3	1:D:438:LEU:HA	1.63	0.81
2:E:281:MET:SD	3:F:64:TRP:HZ2	2.06	0.79
1:A:427:ALA:HB1	2:B:399:ASN:HD22	1.46	0.79
1:A:494:ASN:HD22	1:A:494:ASN:H	1.28	0.78
2:E:283:LYS:NZ	3:F:62:GLU:OE1	2.17	0.77
1:A:494:ASN:HD22	1:A:494:ASN:N	1.82	0.77
3:F:32:ASP:OD1	3:F:33:ASP:N	2.18	0.75
2:E:282:VAL:HG21	2:E:287:LEU:HD11	1.71	0.72
2:E:266:ARG:NH1	3:F:32:ASP:O	2.21	0.72
1:D:467:LYS:HD2	1:D:468:LYS:N	2.03	0.72
2:E:257:ASN:HB3	2:E:260:ILE:HD13	1.71	0.72
2:B:429:THR:HG22	2:B:431:MET:H	1.54	0.72
1:A:467:LYS:HD2	1:A:467:LYS:H	1.56	0.71
2:B:399:ASN:OD1	2:B:399:ASN:N	2.21	0.71
1:A:546:ASN:N	1:A:546:ASN:HD22	1.89	0.71
1:D:448:MET:O	1:D:526:LYS:NZ	2.22	0.71
2:E:257:ASN:OD1	2:E:258:GLN:N	2.23	0.71
1:A:522:GLN:OE1	1:A:522:GLN:HA	1.91	0.69
1:D:336:GLU:HA	1:D:339:HIS:CD2	2.28	0.69
1:D:276:LEU:HD13	1:D:283:LEU:HD12	1.77	0.67
1:A:373:LYS:O	1:A:375:ARG:N	2.27	0.67
1:A:288:ARG:HB2	1:A:337:GLN:HE22	1.61	0.66
1:A:427:ALA:CB	2:B:399:ASN:HD22	2.08	0.66
1:A:349:TYR:CG	1:A:362:GLU:HG3	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:320:HIS:NE2	1:D:533:GLU:OE1	2.29	0.66
1:A:404:ARG:HE	2:B:336:GLU:HB2	1.62	0.65
1:A:291:ARG:HG3	1:A:308:ASN:OD1	1.97	0.64
3:F:75:ASN:H	3:F:75:ASN:HD22	1.46	0.64
1:A:478:GLU:HG3	1:A:489:ILE:HD11	1.77	0.64
1:A:499:GLU:H	1:A:510:THR:HG21	1.61	0.64
2:E:355:THR:HA	2:E:360:GLN:H	1.63	0.64
2:E:380:PHE:CE1	2:E:388:ILE:HG13	2.32	0.64
1:A:285:ASP:HB2	1:A:286:ARG:NH1	2.13	0.63
1:D:335:LEU:O	1:D:338:LEU:HB3	1.99	0.63
1:D:330:SER:CB	1:D:333:GLN:HB2	2.29	0.62
1:A:284:TRP:CZ2	1:A:337:GLN:HG3	2.34	0.62
1:A:256:ARG:HD2	1:A:260:ILE:HD11	1.82	0.62
2:B:244:ASN:HA	2:B:271:MET:HE3	1.80	0.62
1:D:406:ILE:HG12	1:D:453:ILE:HD11	1.82	0.62
1:D:425:PHE:HA	2:E:402:ASN:HD21	1.65	0.61
2:B:172:GLN:N	2:B:172:GLN:OE1	2.33	0.61
1:D:533:GLU:OE2	1:D:537:GLN:NE2	2.32	0.61
3:F:75:ASN:N	3:F:75:ASN:HD22	1.97	0.61
1:D:527:THR:OG1	1:D:528:TYR:N	2.33	0.61
2:E:281:MET:SD	3:F:64:TRP:CZ2	2.91	0.61
3:C:65:ASP:O	3:C:66:ASP:HB2	2.00	0.61
1:D:314:ILE:HG12	1:D:545:ILE:HG12	1.83	0.61
1:D:458:LEU:HD21	1:D:481:LEU:HD11	1.81	0.61
1:A:486:ARG:NH2	1:A:503:GLY:O	2.33	0.61
1:D:339:HIS:CE1	1:D:372:SER:HB2	2.36	0.61
3:F:71:ASP:O	3:F:75:ASN:ND2	2.34	0.60
3:C:56:GLN:HG3	3:C:57:THR:H	1.66	0.60
1:D:326:ASN:HD21	1:D:525:LYS:HZ2	1.49	0.60
2:B:334:LEU:O	2:B:338:LEU:HB2	2.01	0.60
2:E:176:LEU:HB3	2:E:218:GLN:HE21	1.67	0.59
1:D:467:LYS:NZ	1:D:509:LYS:HE2	2.16	0.59
1:A:535:ARG:HG2	1:A:535:ARG:HH11	1.67	0.59
1:D:261:LEU:HD22	1:D:290:ILE:HG23	1.83	0.59
1:D:490:ILE:HG22	1:D:494:ASN:HD21	1.68	0.58
1:D:330:SER:HB3	1:D:333:GLN:HB2	1.85	0.58
1:A:268:ILE:HA	1:A:272:LEU:HD13	1.85	0.58
1:D:326:ASN:HD21	1:D:525:LYS:NZ	2.00	0.58
2:B:282:VAL:HG21	2:B:287:LEU:HD11	1.85	0.58
2:E:401:GLU:O	2:E:405:VAL:HG23	2.03	0.58
1:D:493:CYS:HB3	1:D:498:ILE:HB	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:498:ILE:O	1:D:499:GLU:HB2	2.02	0.58
2:E:266:ARG:HH21	3:F:36:GLU:HG3	1.69	0.57
1:D:256:ARG:NH2	1:D:289:SER:OG	2.36	0.57
2:E:312:GLN:HE21	2:E:377:GLY:HA3	1.69	0.57
2:B:258:GLN:O	2:B:262:ARG:HB2	2.04	0.57
2:E:351:ILE:HG21	2:E:435:ILE:HD13	1.85	0.57
1:A:283:LEU:HD12	1:A:283:LEU:H	1.69	0.57
1:D:340:LYS:HA	1:D:343:ILE:HG12	1.86	0.57
2:E:253:LEU:HD12	2:E:254:PRO:HD2	1.86	0.57
1:D:331:LEU:HD12	1:D:331:LEU:H	1.70	0.57
1:D:472:ILE:HD13	1:D:508:LEU:HG	1.87	0.57
2:B:429:THR:HG22	2:B:431:MET:N	2.20	0.56
2:E:273:PRO:HG3	2:E:299:TRP:CH2	2.41	0.56
1:A:344:THR:O	1:A:348:ILE:HG12	2.06	0.56
1:D:353:ARG:NH2	1:D:362:GLU:OE1	2.38	0.56
1:D:471:PRO:HG3	1:D:501:ILE:HD12	1.88	0.56
1:D:318:ILE:O	1:D:322:MET:HG2	2.05	0.56
2:E:335:LEU:HD21	2:E:390:ILE:HB	1.88	0.56
2:E:452:HIS:N	2:E:452:HIS:ND1	2.53	0.55
1:A:494:ASN:ND2	1:A:494:ASN:N	2.53	0.55
1:D:404:ARG:NH2	2:E:332:ILE:HD13	2.22	0.55
1:A:256:ARG:HB3	1:A:260:ILE:HD11	1.87	0.55
1:A:409:SER:N	1:A:422:CYS:HB2	2.22	0.55
1:A:427:ALA:HB3	2:B:402:ASN:HD22	1.73	0.54
1:A:336:GLU:OE1	1:A:336:GLU:N	2.37	0.54
1:D:339:HIS:HE1	1:D:372:SER:HB2	1.71	0.54
1:D:420:GLU:O	2:E:337:LYS:HD2	2.06	0.54
2:E:183:ASN:HA	2:E:186:TYR:HD2	1.72	0.54
1:D:325:SER:HB2	1:D:327:VAL:HG12	1.90	0.54
1:A:380:ASP:O	1:A:384:GLN:HG3	2.08	0.54
1:A:322:MET:HE2	1:A:329:PHE:HB3	1.90	0.54
1:D:533:GLU:O	1:D:536:LEU:HB3	2.07	0.54
1:A:322:MET:HE3	1:A:327:VAL:HB	1.90	0.54
1:D:348:ILE:O	1:D:352:VAL:HG23	2.08	0.53
1:D:308:ASN:O	1:D:312:VAL:HG23	2.08	0.53
1:A:261:LEU:HD22	1:A:290:ILE:HG12	1.90	0.53
2:B:386:GLN:HE21	2:B:386:GLN:N	2.07	0.53
2:E:272:ILE:HB	2:E:273:PRO:HD3	1.91	0.53
2:E:389:THR:HG23	2:E:391:TYR:H	1.72	0.53
1:D:269:VAL:HG11	1:D:310:ARG:NH2	2.24	0.53
2:B:237:HIS:HA	2:B:278:LEU:HD11	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:CYS:O	1:A:311:ILE:HG13	2.08	0.52
1:D:486:ARG:O	1:D:490:ILE:HG13	2.10	0.52
2:E:251:LEU:HD13	3:F:57:THR:HG21	1.91	0.52
1:D:324:LYS:HD3	1:D:533:GLU:CD	2.30	0.52
1:A:330:SER:C	1:A:332:GLN:H	2.12	0.52
1:D:314:ILE:O	1:D:318:ILE:HG13	2.09	0.52
1:D:326:ASN:ND2	1:D:525:LYS:NZ	2.58	0.51
1:D:504:ASP:OD1	1:D:504:ASP:N	2.42	0.51
1:A:288:ARG:HG2	1:A:292:GLN:HE22	1.75	0.51
1:A:499:GLU:HG2	1:A:510:THR:HG21	1.91	0.51
2:B:388:ILE:HD13	2:B:388:ILE:H	1.75	0.51
1:D:491:GLU:HA	1:D:494:ASN:HD22	1.75	0.51
1:D:452:ASP:HB3	1:D:516:HIS:CD2	2.46	0.51
2:E:379:THR:HG22	2:E:382:ASP:CG	2.31	0.51
2:B:230:TYR:OH	2:B:455:TRP:O	2.20	0.51
1:A:315:HIS:ND1	1:A:334:GLU:OE2	2.38	0.51
2:E:270:TYR:O	2:E:273:PRO:HD2	2.11	0.51
3:C:56:GLN:HG3	3:C:57:THR:N	2.25	0.51
2:E:255:LEU:HD23	2:E:256:THR:H	1.75	0.51
1:D:496:TYR:HD1	1:D:518:LEU:HD21	1.75	0.51
1:A:261:LEU:HD22	1:A:290:ILE:HG23	1.93	0.51
1:A:256:ARG:CZ	1:A:261:LEU:HD21	2.41	0.51
3:F:85:LYS:O	3:F:89:GLN:HG3	2.11	0.51
2:E:263:ASN:HA	2:E:266:ARG:HD2	1.94	0.50
1:A:286:ARG:HH11	1:A:286:ARG:HG2	1.76	0.50
1:D:438:LEU:HD12	1:D:439:PRO:HD2	1.93	0.50
1:A:499:GLU:N	1:A:510:THR:HG21	2.26	0.50
2:B:224:TYR:CZ	2:B:228:ARG:HD2	2.47	0.50
1:A:280:GLU:HA	1:A:283:LEU:HD13	1.93	0.50
1:A:288:ARG:HG2	1:A:292:GLN:NE2	2.28	0.49
3:F:87:GLU:O	3:F:89:GLN:N	2.44	0.49
2:E:200:LYS:HD2	2:E:203:GLN:HE22	1.77	0.49
2:B:335:LEU:HD21	2:B:390:ILE:HB	1.93	0.49
1:A:427:ALA:CB	2:B:402:ASN:HD22	2.25	0.49
1:A:475:ILE:H	1:A:475:ILE:HD12	1.77	0.49
1:D:467:LYS:C	1:D:467:LYS:HD2	2.32	0.49
1:A:427:ALA:H	2:B:402:ASN:ND2	2.11	0.49
1:A:288:ARG:CB	1:A:337:GLN:HE22	2.24	0.49
1:D:404:ARG:HD2	2:E:336:GLU:HB2	1.94	0.49
1:D:496:TYR:CD1	1:D:518:LEU:HD21	2.47	0.49
1:D:337:GLN:HA	1:D:340:LYS:HG3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:332:GLN:NE2	1:D:333:GLN:HA	2.28	0.49
1:A:405:VAL:HG22	1:A:425:PHE:HB2	1.93	0.49
1:D:380:ASP:OD1	1:D:404:ARG:NH2	2.39	0.49
1:D:403:ARG:HB2	1:D:404:ARG:NH1	2.28	0.49
2:B:348:LYS:HB2	2:B:436:VAL:HG11	1.94	0.49
2:B:244:ASN:HA	2:B:271:MET:CE	2.41	0.49
2:E:333:VAL:O	2:E:337:LYS:HG2	2.13	0.49
1:A:332:GLN:C	1:A:334:GLU:H	2.16	0.49
1:D:404:ARG:HH21	2:E:332:ILE:CG2	2.25	0.48
1:A:409:SER:H	1:A:422:CYS:HB2	1.78	0.48
1:D:345:LEU:HD22	1:D:349:TYR:CZ	2.48	0.48
1:A:322:MET:CE	1:A:329:PHE:HB3	2.43	0.48
1:D:474:PHE:O	1:D:478:GLU:HG3	2.12	0.48
2:E:351:ILE:HD13	2:E:435:ILE:HD11	1.94	0.48
2:B:344:ARG:HH11	2:B:344:ARG:HG2	1.78	0.48
1:D:337:GLN:HA	1:D:340:LYS:CG	2.44	0.48
2:E:336:GLU:OE1	2:E:337:LYS:HE3	2.13	0.48
1:D:498:ILE:HG12	1:D:511:LEU:HD13	1.96	0.48
1:D:427:ALA:O	1:D:431:GLN:HG3	2.13	0.48
1:D:382:ASN:N	1:D:382:ASN:HD22	2.12	0.48
1:A:343:ILE:O	1:A:347:GLU:HG3	2.14	0.48
2:E:277:ILE:HD11	2:E:334:LEU:HD23	1.96	0.47
2:E:312:GLN:HG2	2:E:316:LEU:HD13	1.96	0.47
2:B:388:ILE:HD13	2:B:388:ILE:N	2.28	0.47
1:A:351:ASP:OD1	1:A:351:ASP:N	2.46	0.47
3:C:55:THR:OG1	3:C:56:GLN:N	2.43	0.47
3:C:71:ASP:HA	3:C:75:ASN:ND2	2.29	0.47
1:A:507:ASP:O	1:A:510:THR:HG22	2.14	0.47
2:E:354:TRP:HD1	2:E:355:THR:HG22	1.79	0.47
2:E:200:LYS:HD2	2:E:203:GLN:NE2	2.29	0.47
1:A:402:PHE:O	1:A:406:ILE:HG13	2.15	0.47
1:A:373:LYS:HA	1:A:373:LYS:HE2	1.96	0.47
2:B:401:GLU:O	2:B:405:VAL:HG23	2.14	0.47
1:D:412:THR:HG22	1:D:418:LYS:HE2	1.96	0.47
1:A:332:GLN:HB3	1:A:335:LEU:HG	1.97	0.47
1:D:428:ARG:HD3	2:E:393:GLY:O	2.15	0.47
2:B:349:THR:HG21	3:C:77:LEU:HD23	1.97	0.47
1:A:353:ARG:NH1	1:A:387:PRO:HG2	2.30	0.47
2:E:268:LEU:O	2:E:272:ILE:HG12	2.15	0.47
3:C:62:GLU:CD	3:C:62:GLU:H	2.17	0.47
1:A:372:SER:HA	1:A:445:PHE:CZ	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:429:THR:HG23	2:E:431:MET:H	1.78	0.47
1:D:370:LEU:HD23	1:D:379:TYR:HB3	1.96	0.46
1:D:343:ILE:O	1:D:347:GLU:HG2	2.16	0.46
1:A:353:ARG:CZ	1:A:387:PRO:HG2	2.46	0.46
2:E:200:LYS:HB3	2:E:200:LYS:HE3	1.78	0.46
1:A:257:PRO:HD2	1:A:260:ILE:HG12	1.97	0.46
1:A:256:ARG:NH2	1:A:289:SER:OG	2.49	0.46
2:E:280:LYS:HG3	2:E:440:ASN:HD22	1.81	0.46
1:A:258:PRO:HA	1:A:294:PHE:CE1	2.50	0.46
1:D:364:GLU:HG2	1:D:368:TYR:CE2	2.51	0.46
1:D:263:LYS:HA	1:D:266:ASP:HB2	1.98	0.46
3:F:56:GLN:HB3	3:F:57:THR:H	1.50	0.46
2:E:307:ARG:HH11	2:E:307:ARG:HG2	1.81	0.46
1:A:361:ASN:HD21	1:A:548:GLY:HA3	1.80	0.46
2:B:254:PRO:O	2:B:256:THR:N	2.43	0.45
1:D:467:LYS:HZ3	1:D:509:LYS:HE2	1.80	0.45
3:C:57:THR:O	3:C:59:ILE:HG23	2.16	0.45
1:D:467:LYS:HZ2	1:D:509:LYS:HE2	1.81	0.45
2:B:288:ARG:N	2:B:289:PRO:HD2	2.32	0.45
2:B:312:GLN:OE1	2:B:378:PRO:HD2	2.16	0.45
1:D:326:ASN:ND2	1:D:525:LYS:HZ3	2.13	0.45
1:D:268:ILE:HG23	1:D:283:LEU:HD22	1.99	0.45
1:A:380:ASP:CG	1:A:403:ARG:HH21	2.19	0.45
1:D:382:ASN:HD22	1:D:382:ASN:H	1.65	0.45
3:F:68:GLU:HG2	3:F:74:THR:HG21	1.98	0.45
2:E:273:PRO:HB3	2:E:334:LEU:HD21	1.98	0.45
1:A:287:MET:HB3	1:A:311:ILE:HD13	1.98	0.45
2:E:404:LEU:O	2:E:408:ILE:HG13	2.17	0.45
2:E:312:GLN:NE2	2:E:377:GLY:HA3	2.30	0.45
1:D:383:ILE:HD12	1:D:386:LEU:HD12	1.99	0.45
2:E:355:THR:HG22	2:E:360:GLN:O	2.17	0.44
2:B:199:PHE:HB3	2:B:455:TRP:HA	1.99	0.44
2:B:273:PRO:HB3	2:B:299:TRP:CH2	2.51	0.44
1:D:264:THR:O	1:D:268:ILE:HG13	2.17	0.44
1:D:297:GLN:HE21	1:D:297:GLN:HB2	1.67	0.44
1:A:546:ASN:ND2	1:A:546:ASN:N	2.61	0.44
1:D:262:VAL:HG12	1:D:266:ASP:OD2	2.18	0.44
1:A:299:TYR:HE2	1:A:303:GLU:HB2	1.82	0.44
2:E:266:ARG:NH2	3:F:36:GLU:HG3	2.32	0.44
1:A:532:LEU:HA	1:A:535:ARG:HD3	1.99	0.44
1:D:535:ARG:HG2	1:D:535:ARG:HH11	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:302:LEU:HB2	2:B:317:TRP:CE2	2.52	0.44
2:E:380:PHE:CD1	2:E:380:PHE:C	2.90	0.44
1:D:330:SER:HB2	1:D:333:GLN:HB2	1.97	0.44
2:E:312:GLN:NE2	2:E:378:PRO:HD2	2.33	0.44
2:E:216:LEU:O	2:E:220:ILE:HG13	2.17	0.44
2:B:284:TRP:O	2:B:288:ARG:HG3	2.17	0.44
2:B:344:ARG:HG2	2:B:344:ARG:NH1	2.33	0.43
2:E:280:LYS:HG3	2:E:440:ASN:ND2	2.33	0.43
1:D:513:HIS:CD2	1:D:518:LEU:CD2	2.94	0.43
2:B:308:TYR:OH	3:C:68:GLU:O	2.20	0.43
2:B:251:LEU:HA	2:B:255:LEU:HD21	1.99	0.43
3:F:75:ASN:N	3:F:75:ASN:ND2	2.65	0.43
1:A:329:PHE:N	1:A:329:PHE:CD1	2.86	0.43
1:A:428:ARG:HA	1:A:431:GLN:OE1	2.18	0.43
1:A:261:LEU:HD23	1:A:261:LEU:HA	1.78	0.43
1:A:258:PRO:HA	1:A:294:PHE:CZ	2.54	0.43
2:B:368:ILE:HD12	2:B:404:LEU:HD11	2.00	0.43
2:B:308:TYR:OH	3:C:69:VAL:HA	2.19	0.43
1:D:420:GLU:HB3	2:E:447:PHE:CD2	2.53	0.43
2:B:319:ARG:HA	2:B:391:TYR:CZ	2.53	0.43
1:A:378:GLN:O	1:A:381:GLU:HB3	2.19	0.43
2:B:222:TYR:CE1	2:B:454:LEU:HB3	2.54	0.43
1:A:288:ARG:HB2	1:A:337:GLN:NE2	2.31	0.42
2:E:232:LEU:CD2	2:E:329:GLN:HG2	2.49	0.42
1:A:288:ARG:O	1:A:292:GLN:HB2	2.19	0.42
2:E:356:THR:HG22	2:E:429:THR:O	2.20	0.42
1:A:291:ARG:O	1:A:295:THR:HG23	2.19	0.42
1:D:403:ARG:CB	1:D:404:ARG:NH1	2.83	0.42
2:E:372:LEU:HD11	2:E:403:VAL:HG11	2.01	0.42
1:D:470:LYS:HA	1:D:471:PRO:HD2	1.73	0.42
2:E:283:LYS:O	2:E:286:PRO:HD2	2.20	0.42
1:D:336:GLU:O	1:D:340:LYS:HG2	2.20	0.42
2:E:354:TRP:NE1	2:E:360:GLN:HB3	2.34	0.42
1:D:458:LEU:HD21	1:D:481:LEU:CD1	2.45	0.42
1:A:427:ALA:HB1	2:B:399:ASN:ND2	2.25	0.42
1:D:452:ASP:HB3	1:D:516:HIS:HD2	1.82	0.42
2:B:284:TRP:CD2	2:B:296:ILE:HG23	2.54	0.42
2:E:244:ASN:HA	2:E:271:MET:CE	2.49	0.42
2:B:230:TYR:CD2	2:B:238:ASN:HB3	2.54	0.42
1:A:381:GLU:HG3	2:B:329:GLN:OE1	2.20	0.41
1:A:498:ILE:HD11	1:A:511:LEU:HD22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:354:TRP:O	2:E:360:GLN:HB2	2.20	0.41
1:D:404:ARG:HH21	2:E:332:ILE:HG21	1.85	0.41
1:A:420:GLU:HG3	2:B:447:PHE:CG	2.54	0.41
1:A:404:ARG:NE	2:B:336:GLU:OE1	2.54	0.41
1:D:443:GLY:O	1:D:447:GLN:HG3	2.20	0.41
1:A:433:MET:HE1	1:A:438:LEU:HD21	2.01	0.41
1:A:404:ARG:HH11	1:A:404:ARG:HD3	1.76	0.41
1:A:474:PHE:O	1:A:478:GLU:HB2	2.20	0.41
1:D:454:ARG:HG2	1:D:481:LEU:HD22	2.01	0.41
2:E:203:GLN:HB3	2:E:455:TRP:CZ2	2.56	0.41
2:B:171:LYS:HA	2:B:171:LYS:HD2	1.47	0.41
2:E:237:HIS:HA	2:E:278:LEU:HD11	2.02	0.41
2:E:380:PHE:HE1	2:E:386:GLN:O	2.03	0.41
1:A:285:ASP:HB2	1:A:286:ARG:HH12	1.86	0.41
2:E:450:HIS:CG	2:E:451:SER:N	2.89	0.41
3:F:62:GLU:HG2	3:F:63:ASN:N	2.35	0.41
2:E:268:LEU:HD13	2:E:287:LEU:HD13	2.02	0.41
1:A:508:LEU:HA	1:A:508:LEU:HD23	1.91	0.41
1:A:395:LEU:HD13	1:A:395:LEU:HA	1.79	0.41
1:A:324:LYS:HE2	1:A:533:GLU:HG3	2.03	0.41
1:A:447:GLN:OE1	1:A:532:LEU:HD12	2.20	0.41
1:D:286:ARG:O	1:D:290:ILE:HG13	2.21	0.41
1:A:329:PHE:O	1:A:330:SER:HB3	2.21	0.41
2:E:319:ARG:HA	2:E:391:TYR:CZ	2.56	0.41
2:E:453:VAL:HG13	2:E:455:TRP:CE2	2.56	0.41
1:A:433:MET:HE3	1:A:446:LEU:HD13	2.02	0.41
2:E:348:LYS:HB2	2:E:436:VAL:HG11	2.03	0.41
2:B:435:ILE:HG12	2:B:435:ILE:H	1.73	0.41
2:B:304:LYS:HD3	3:C:70:ASP:HB2	2.01	0.41
1:D:472:ILE:HD12	1:D:472:ILE:N	2.36	0.40
1:A:336:GLU:O	1:A:340:LYS:N	2.43	0.40
1:A:267:TYR:CE2	1:A:272:LEU:HD11	2.57	0.40
3:F:54:VAL:O	3:F:56:GLN:N	2.54	0.40
2:E:440:ASN:O	2:E:444:THR:HG23	2.22	0.40
1:A:428:ARG:HA	1:A:431:GLN:HB2	2.02	0.40
1:A:324:LYS:HG3	1:A:533:GLU:OE1	2.21	0.40
2:E:338:LEU:HA	2:E:338:LEU:HD23	1.86	0.40
2:B:358:TRP:CE3	3:C:85:LYS:HD3	2.57	0.40
1:A:345:LEU:HD22	1:A:349:TYR:CZ	2.57	0.40
1:D:349:TYR:CG	1:D:362:GLU:HG3	2.57	0.40
1:D:365:PHE:HA	1:D:368:TYR:HD2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:193:GLN:N	2:E:193:GLN:OE1	2.54	0.40

All (1) 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)
3:C:86:ARG:NH2	3:F:38:PHE:O[5_445]	2.18	0.02

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	297/299 (99%)	273 (92%)	19 (6%)	5 (2%)	11	43
1	D	297/299 (99%)	266 (90%)	23 (8%)	8 (3%)	6	31
2	B	284/286 (99%)	261 (92%)	22 (8%)	1 (0%)	39	75
2	E	284/286 (99%)	258 (91%)	24 (8%)	2 (1%)	26	65
3	C	45/60 (75%)	33 (73%)	8 (18%)	4 (9%)	1	5
3	F	45/60 (75%)	36 (80%)	5 (11%)	4 (9%)	1	5
All	All	1252/1290 (97%)	1127 (90%)	101 (8%)	24 (2%)	10	40

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	374	ILE
3	C	56	GLN
3	C	71	ASP
1	D	468	LYS
1	D	499	GLU
3	F	56	GLN
1	A	254	ASP

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Mol	Chain	Res	Type
1	A	531	CYS
3	C	68	GLU
1	D	519	SER
2	B	255	LEU
1	D	331	LEU
2	E	380	PHE
3	F	55	THR
3	F	87	GLU
3	F	88	ASN
1	A	258	PRO
1	A	279	SER
1	D	471	PRO
2	E	398	LYS
3	C	55	THR
1	D	360	PRO
1	D	498	ILE
1	D	305	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	278/278 (100%)	263 (95%)	15 (5%)	27	64
1	D	278/278 (100%)	264 (95%)	14 (5%)	30	67
2	B	265/265 (100%)	253 (96%)	12 (4%)	34	70
2	E	265/265 (100%)	257 (97%)	8 (3%)	48	81
3	C	47/56 (84%)	44 (94%)	3 (6%)	22	57
3	F	47/56 (84%)	46 (98%)	1 (2%)	61	86
All	All	1180/1198 (98%)	1127 (96%)	53 (4%)	34	70

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	260	ILE

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Mol	Chain	Res	Type
1	A	286	ARG
1	A	292	GLN
1	A	297	GLN
1	A	329	PHE
1	A	404	ARG
1	A	405	VAL
1	A	428	ARG
1	A	445	PHE
1	A	459	ARG
1	A	467	LYS
1	A	494	ASN
1	A	522	GLN
1	A	540	THR
1	A	546	ASN
2	B	172	GLN
2	B	206	SER
2	B	248	GLN
2	B	307	ARG
2	B	321	ASN
2	B	333	VAL
2	B	347	ILE
2	B	386	GLN
2	B	388	ILE
2	B	399	ASN
2	B	435	ILE
2	B	439	VAL
3	C	57	THR
3	C	74	THR
3	C	75	ASN
1	D	263	LYS
1	D	286	ARG
1	D	297	GLN
1	D	325	SER
1	D	331	LEU
1	D	337	GLN
1	D	340	LYS
1	D	382	ASN
1	D	404	ARG
1	D	445	PHE
1	D	470	LYS
1	D	513	HIS
1	D	527	THR

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Mol	Chain	Res	Type
1	D	533	GLU
2	E	173	ARG
2	E	218	GLN
2	E	324	HIS
2	E	347	ILE
2	E	388	ILE
2	E	429	THR
2	E	435	ILE
2	E	452	HIS
3	F	75	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	292	GLN
1	A	297	GLN
1	A	332	GLN
1	A	337	GLN
1	A	494	ASN
1	A	546	ASN
2	B	252	ASN
2	B	305	HIS
2	B	386	GLN
2	B	402	ASN
2	B	416	ASN
3	C	75	ASN
3	C	89	GLN
1	D	326	ASN
1	D	332	GLN
1	D	339	HIS
1	D	378	GLN
1	D	382	ASN
1	D	434	GLN
1	D	494	ASN
2	E	203	GLN
2	E	215	GLN
2	E	218	GLN
2	E	238	ASN
2	E	312	GLN
2	E	329	GLN
2	E	402	ASN
2	E	433	GLN

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Mol	Chain	Res	Type
3	F	75	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](#)

1 ligand is 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	$\# Z > 2$
4	SO4	A	601	-	4,4,4	0.38	0	6,6,6	0.19	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
4	SO4	A	601	-	-	0/0/0/0	0/0/0/0

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

There are no such residues in this entry.

5.8 Polymer linkage issues

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	299/299 (100%)	-0.37	2 (0%) 89 78	34, 65, 115, 169	0
1	D	299/299 (100%)	-0.20	0 100 100	50, 94, 139, 165	0
2	B	286/286 (100%)	-0.56	1 (0%) 94 88	30, 50, 83, 154	0
2	E	286/286 (100%)	-0.32	1 (0%) 94 88	40, 71, 110, 152	0
3	C	49/60 (81%)	-0.37	0 100 100	45, 81, 138, 158	0
3	F	49/60 (81%)	-0.21	1 (2%) 68 46	56, 100, 157, 180	0
All	All	1268/1290 (98%)	-0.35	5 (0%) 93 85	30, 72, 127, 180	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	170	GLY	3.4
1	A	253	SER	2.5
3	F	64	TRP	2.3
1	A	254	ASP	2.2
2	E	435	ILE	2.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	SO4	A	601	5/5	0.96	0.12	-1.65	88,90,96,107	0

6.5 Other polymers [i](#)

There are no such residues in this entry.